MCA-08 / BCA-12: Computer Oriented Numerical Methods

Page no:

Block 1:	Introduction	4
Unit 1:	Computer Arithmetic and Solution of Non-Linear Equations	5
Block 2:	Various methods of Algebraic Equations	26
Unit 2:	Solution of Linear Algebraic Equations	27
Block 3:	Interpolation Concepts	52
Unit 3:	Interpolation and curve Fitting	53
Block 4:	Differentiation and integration methods	84
Unit 4:	Numerical Differentiation and Integration	85

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Course introduction

This book provides a complete guide for the implementation of Computer oriented numerical methods concepts. This book is very much helpful for you career development in the IT industries, so Computer oriented numerical methods is very much essential in this competitive world. There are large numbers of examples, model questions, objectives, summaries of important topics and learning activities are available in this book, which are very much useful for universities and job oriented examinations of various reputed companies. It is very useful for BCA, MCA and PGDCA student of Universities, computer institutions and so on.

This book covers four blocks and we discussed many topics with detailed explanation for each blocks; Block one deal with computer arithmetic and solution of non-linear equations, block two deals with solution of linear algebraic equations, block three deals with interpolation and curve fitting and finally block four deals with numerical differentiation and integration.

Most of the concepts in the text are illustrated by several examples are important topics in their own right and may be treated as such. We feel that, at the stage of a student's development for which the test is designed, it is more important to cover several examples in great detail than to cover a broad range of topics cursorily. All the formulas and theorems in this text have been tested and debugged. Of course, any errors that remain are the sole responsibility of the course writer.

We have tried the best to avoid the mistakes and errors, however their presence cannot be ruled out. Your valuable suggestions and corrections are welcomed to improve our quality. This book is dedicated to all of our students and colleagues.

Block 1: Introduction

In this block, we will learn about the computer arithmetic and solution of non linear equations. In this we get the knowledge of Newton Raphson method, Regula falsi method, secant method and etc. this block is divided into one unit are as follows.

Unit 1: it deals with computer arithmetic and non-linear solutions.

UNIT-1

COMPUTER ARITHMETIC AND SOLUTION OF NON-LINEAR EQUATIONS

Structure

Overview

Learning Objectives

1.1. Floating Point Represent of Numbers

1.2. Sources of Errors

1.3. Non-Associativity of Arithmetic

1.4 Propagated Errors

1.5 Pitfalls in Computation

1.6 Solution of Non-Linear Equations

1.7 The Bisection Method

1.8 Fixed point iteration

1.9 Regular Falsi Method

1.10 Newton's Raphson Method

1.11 Secant Method

1.12 Convergence Criteria of Iterative Method

Keywords

Answer to Learning Activities

References

OVERVIEW

A computer is a device or machine for making calculations or controlling operations that are expressible in numerical or logical terms. It is nothing but a system accepting input from a user process the same, and giving the output in the required format. It is capable of manipulating numbers and symbols under the control of set instructions known as a computer program.

In order to write computer program without any logical error, it is recommended programmers prepare a rough writing showing the steps involved in the program. This is called an algorithm. An algorithm presents step-by-step instructions required to solve any problem.

The main feature of computer, which influence the formulation of algorithm. Formulation of algorithm is the main subject matter of the *Numerical Analysis.*

LEARNING OBJECTIVES

After studying this unit, you should be able to discuss about

- Explain the concepts of Floating Point Arithmetic Operations
- Discuss the sources of errors
- Explain the concept of pitfalls in Computation
- To find solution of non linear equations using Bisection, Fixed Point, Regular Falsi, Newton's Raphson and Second Method.
- Discuss Convergence criteria of Iterative Methods

1.1 FLOATING POINT REPRESENT OF NUMBERS

Computers have both an integer mode and a floating point mode for representing numbers. The integer mode is used for performing calculations that are known to be integer value and have limited usage for *numerical analysis.* Floating point numbers are used for scientific and engineering applications. Computers represent floating point numbers in binary form.

For generality, they use a binary form of scientific notation.

In standardized base 10 notation, $29.25 = 0.2925 \times 10^3$.

In binary notation, $29.25 = 11101.01_{(2)} = 0.1110101_{(2)} \times 2^5$.

Computer has standard format of floating point numbers:

Precision	Number of Bits	Bits for Mantissa	Exponent	Range	Decimal Digits
Single	32	24	8	2^{-128} to 2^{127}	6
Single	48	40	8	2^{-128} to 2^{127}	11
Double	64	53	11	2^{-1024} to 2^{1023}	16

Floating Point Arithmetic Operations: The floating point arithmetic operations are addition, subtraction multiplication and division.

Addition: If exponents are equal then sum of two floating point number,

Case 1:

Let $a = .4516E3$ and $b = .5433E3$,

$$\begin{array}{r} .4516 \\ +\ .5433 \\ \hline .9949 \\ \hline \end{array}$$

The sum of *a* and *b* is .9919*E*3

Case 2:

Let $a = .4616E3$ and $b = .6533E3$ then sum of *a* and *b* is,

$$\begin{array}{r} .4616E3 \\ +\ .6533E3 \\ \hline 1.1149E3 \\ \hline \end{array}$$

Here 1.1149E3 can be written as .1114E4.

i.e., the exponent is increased by one and the last digit of the mantissa is chopped off. The sum of a and b is .1114E4.

If exponents are unequal then sum of two floating point number, $a = .4616E3$ and $b = .6533E5$, here exponent of a is smaller than b and then the exponent of a is shifted right by a number of places equal to the difference in the two exponents and hence

a = .0046E5.

$$\begin{array}{r} .0046E5 \\ +\ .6533E5 \\ \hline .6579E5 \\ \hline \end{array}$$

Thus the answer would be .6579E5

Similarly, if $a = .4616E3$ and $b = .6533E7$ then,

$$\begin{array}{r} .0000E7 \\ +\ .6533E7 \\ \hline .6533E7 \\ \hline \end{array}$$

Here a is will be shifted 4 places to the right i.e., a = .0000E7. The answer would be .6533E7.

Subtraction: If exponents are equal then subtraction of two floating point number, let $a = .4341E3$ and $b = .4232E3$ then subtract b from a,

$$\begin{array}{r} .4341E3 \\ +\ .4232E3 \\ \hline .0109E3 \\ \hline \end{array}$$

Then answer of a - b is .0109E3

If exponents are unequal, if $a = .4543E-3$ and $b = .8341E-4$, subtract *b* from *a*. Here exponent of *b* is smaller than *a*, then the exponent of *b* is shifted right and exponent increased by one for each right digit.

Hence, $b = .0834E-3$.

$$
\begin{array}{r}
.4543E - 3 \\
+\ .0834E - 3 \\
\hline
.3709E - 3 \\
\hline
\end{array}
$$

Thus the answer would be $.3709E-5$.

Multiplication: Two numbers are multiplied in the normalized floating point mode by multiplying the mantissa and adding the exponents.

If $a = .7232E13$ and $b = .2342E-15$,

$a \times b = 0.16937344E-2$

$= 0.1693E-2$.

If $a = .4212E13$ and $b = .1231E-15$,

$a \times b = 0.05184972E-2$

$= 0.0518E-2$

$= 0.5180E-1$

Division: Two numbers are divided in the normalized floating point mode by dividing the mantissa of the numerator by the denominator. The denominator exponent is subtracted from the numerator exponent.

if $a = .2222E-17 \,\&\, b = .1010E-10$ then

$\frac{a}{b} = 2.2000E-7 = .2200E-5$.

1.2 SOURCES OF ERRORS

When using numerical algorithms, we try to

- Minimize numerical errors in computation
- Recognize unavoidable errors and
- (if possible, reduce computation time)

The most common ways errors enter numerical calculations are

- Round off error (finite representation of numbers)
- Truncation error (approximating complicated functions with simpler ones in calculations)
- Error in input (finite accuracy of measured inputs) and
- Bugs in software.

1.3 NON-ASSOCIATIVITY OF ARITHMETIC

Consequence of the floating point is that the associative and distributive laws of arithmetic are not always valid.

$$ie., (a+b)-c \neq (a-c)+b$$
$$a(b-c) \neq (ab-ac)$$

These are illustrated with examples below.

Let $a = .4554E1$

$b = .4445E - 1$

$c = .4543E1$

$$(a+b) = .4554E1 + .4445E-1$$
$$= .4554E1 + .0044E1$$
$$= .4598E1$$

$$(a+b)-c = .4598E1 - .4543E1$$
$$= .0055E1$$
$$= .5500E-1$$

$$
\begin{aligned}
(a-c) &= .4554E1 - .4543E1 \\
&= .0055E1 \\
&= .1100E-1
\end{aligned}
$$

$$
\begin{aligned}
(a-c)+b &= .1100E-1 + .4445E-1 \\
&= .5545E-1
\end{aligned}
$$

$\therefore (a+b)-c \neq (a-c)+b$ (Associative Law is not valid)

Let $a = .5555E1$

$b = .4545E1$

$c = .4535E1$

$$(b-c) = .0010E1 = .1000E-1$$

$$
\begin{aligned}
a(b-c) &= .5555E1 \times .1000E-1 \\
&= .0555E0 \\
&= .5550E-1
\end{aligned}
$$

$$
\begin{aligned}
ab &= .5555E1 \times .4545E1 \\
&= .2524E2
\end{aligned}
$$

$$
\begin{aligned}
ac &= .5555E1 \times .4535E1 \\
&= .2519E2
\end{aligned}
$$

$$ab - ac = .0005E2 = .5000E-1$$

$\therefore a(b-c) \neq ab - ac.$ (Distributive Law is not valid).

1.4 PROPAGATED ERRORS

Propagation of errors:

Let ω denote one of the arithmetic operations +,-,×, / and ω^* be the corresponding computer version including rounding. $x_A, y_A \in A$ are numbers being used for calculation, and x_T, y_T are true(real) numbers. And let $\varepsilon := x_A - x_T$, $\eta := y_A - y_T$. Then

$$x_A w^* y_A - x_T w y_T = \underbrace{x_A w y_A - x_T w y_T}_{\text{propagated error}} + \underbrace{x_A w^* y_A - x_A w y_A}_{\text{rounding or chopping error}}$$

If an exact rounding is used

$$|x_A w^* y_A - x_A w y_A| \leq (x_A w y_A)\beta^{1-t}/2$$

Or

$$x_A \omega^* y_A = x_A \omega y_A (1+\delta)$$

Rounding; $|\delta| \le \beta^{1-t}/2$, chopping; $|\delta| \le \beta^{1-t}$

Propagated Errors

1. **Multiplicative case:**

$$x_A y_A - x_T y_T = (x_T+\varepsilon)(y_T+\eta) - x_T y_T = x_T\eta + y_T\varepsilon + \varepsilon\eta$$

$$Rel(x_T \times y_T) = \frac{x_T\eta + y_T\varepsilon + \varepsilon\eta}{x_T \times y_T} \simeq \frac{\eta}{y_T} + \frac{\varepsilon}{x_T} = Rel(x_A) + Rel(y_A)$$

2. **Division case :**

$$Rel(x_T/y_T) = \frac{x_A/y_A - x_T/y_T}{x_T/y_T} = \frac{(x_T+\varepsilon)/(y_T+\eta) - x_T/y_T}{x_T/y_T} \simeq \frac{x_T(1+\tilde{\varepsilon})/y_T(1+\tilde{\eta}) - x_T/y_T}{x_T/y_T}$$

$$= \frac{(1+\tilde{\varepsilon}) - (1+\tilde{\eta})}{1+\tilde{\eta}} \simeq \tilde{\varepsilon} - \tilde{\eta} = Rel(x_A) - Rel(y_A)$$

3. **Addition and subtraction:**

$$(x_A \pm y_A) - (x_T \pm y_T) = \varepsilon \pm \eta$$

$$Rel(x_A \pm y_A) = \frac{\varepsilon \pm \eta}{x_T \pm y_T}$$

$\boldsymbol{Rel}(x_A \pm y_A)$ may be extremely large if $x_T \pm y_T$ is small(overflow).

Relative errors for multiplicative and division *do not* propagate rapidly but those for *addition* and *subtraction* may propagate rapidly.

1.5 PITFALLS IN COMPUTATION

When the result of a floating-point operation is not representable as a normalized floating point number, and exception occurs. A main contribution of Computer Arithmetic was to standardize on how exceptions are handled. There are five kinds of exceptions, as listed in the table below.

S. No.	Exception Name	Cause	Default Result
1	Overflow	Result too large to represent as a normalized number	Return + (- Infinity)
2	Underflow	Result too small to represent as a nonzero normalized number	Return subnormal number or 0
3	Divide-by-zero	Computing x/0, where x is finite and nonzero	Return + (- infinity)
4	Invalid	Infinity-infinity, 0*infinity, infinity/infinity, 0/0, sqrt (-1), x rem 0, infinity rem y, comparison with NAN, impossible binary-decimal conversion	NAN
5	Inexact	A rounding error occurred	rounded result

1.6 SOLUTION OF NON-LINEAR EQUATIONS

Non-Linear Equation: A non-linear equation is an equation containing a transcendental function (non-linear functions). Examples of such an equation are

$$x - \sin x - e^{x} = 0$$

$$x^{2} \log x - 2 \log x + 1 = 0$$

Some methods of finding solutions to a transcendental equation (Non-Linear equation) use Bisection, Regular False, Fixed Point, Newton Raphson and Secant Method.

1.7 THE BISECTION METHOD

Bisection Method: If $f(x)$ is real and continuous in the interval from x_0 to b and $f(x_0)$ and $f(x_1)$ have opposite signs,

That is: $f(x_0) * f(x_1) < 0$

There is at least one root in the equation.

A new root estimate can be determined by:

$$x_2 = \frac{x_0 + x_1}{2}$$

Having the value for the root 3 cases are possible:

1. if $f(x_2) > 0$ and we make $x_1 = x_2$
2. if $f(x_2) < 0$ and we make $x_0 = x_2$
3. if $f(x_2) = 0$ and c is the exact root.

In this new interval we again calculate $f(x_2)$. Calculation will stop when the maximum iterations number is reached or we terminate the process if two consecutive iteration values are nearly equal.

Example 1.1

Find the largest root of $f(x) = x^6 - x - 1 = 0$ for $x = 1$ and $x = 2$ using Bisection method.

Solution:

We choose $x_0 = 1$ and $x_1 = 2$.

Let $f(x) = x^6 - x - 1 = 0$

Then $f(x_0) = -1$ and $f(x_1) = 61$ requirement $f(x_0)\ f(x_1) < 0$ is satisfied.

Therefore $x_2 = \frac{x_0 + x_1}{2}$ = 1.5000

The results from Bisect are shown in the table.

The entry n indicates the iteration number n.

N	x_0	x_1	X_2	$f(x_2)$
1	1.0000	2.0000	1.5000	8.8906
2 $(x_1 \leftarrow x_2)$	1.0000	1.5000	1.2500	1.5647
3 $(x_1 \leftarrow x_2)$	1.0000	1.2500	1.1250	-0.0977
4 $(x_0 \leftarrow x_2)$	1.1250	1.2500	1.1875	0.6167
5 $(x_1 \leftarrow x_2)$	1.1250	1.1875	1.1562	0.2333
6 $(x_1 \leftarrow x_2)$	1.1250	1.1562	1.1406	0.0616
7 $(x_1 \leftarrow x_2)$	1.1250	1.1406	1.1328	-0.0196
8 $(x_0 \leftarrow x_2)$	1.1328	1.1406	1.1367	0.0206
9 $(x_1 \leftarrow x_2)$	1.1328	1.1367	1.1348	0.0004
10 $(x_1 \leftarrow x_2)$	1.1328	1.1348	**1.1338**	**-0.0094**

Here $f(x_2)$ = -0.0096 when x_2 is 1.1338.

Therefore, root is approximately **1.1338**

Advantages:

1. It always converges.
2. You have a guaranteed error bound, and it decreases with each successive iteration.
3. You have a guaranteed rate of convergence. The error bound decreases by ½ with each iteration.

Disadvantages:

1. It is relatively slow when compared with other root finding methods.
2. If one of the initial guesses is closer to the root, it will take larger number of iterations to reach the root.

1.8 FIXED POINT ITERATION

Fixed Point Iteration: Fixed point iteration is a method of computing fixed points of functions. More specifically, given a function *f* defined on the real numbers with real values (or, more generally, defined on a metric space with values in itself) and given a point x_0 in the domain of *f*, the fixed point iteration is $x_{n+1} = f(x_n), n = 0,1,2,...$ which gives rise to the sequence $x_0, x_1, x_2,...$ which is hoped to converge to a point *x*. If *f* is continuous, then one can prove that the obtained *x* is a fixed point of *f*.

Example 1.2

Find the root of the equation $x^3 + x + 1 = 0$, using fixed point iteration.

Solution:

Let $f(x) = x^3 + x + 1 = 0$

f(-1) < 0 and *f*(0) > 0. Therefore, the root lies between –1 and 0.

$$x^3 + x + 1 = 0$$

i.e., $x^3 + x = -1$

i.e., $x^2(x+1) = -1$

i.e., $x = -\dfrac{1}{x^2+1}$

The equation can be written as $x = -\dfrac{1}{x^2+1}$, so that it takes the form $x_{n+1} = f(x_n), n = 0,1,2,...$.

Take x_0 = -1. Then $x_1 = -\dfrac{1}{x_0^2+1} = -0.5$.

The iteration are,

Iteration (n)	x_n	$f(x_n) = -\frac{1}{x_n^2+1} = x_{n+1}$	$x_{n+1}^3 + x_{n+1} + 1$
0	-1	-0.5000	0.375
1	-0.5	-0.8000	-0.312
2	-0.8	-0.6097	0.1636
3	-0.6097	-0.7290	-0.116
4	-0.729	-0.6529	0.068
5	-0.6529	-0.7010	-0.045
6	-0.701	-0.6705	0.028
7	-.6705	-0.6898	-0.018
8	-0.6898	-0.6775	0.011
9	-0.6775	-0.6853	-0.007
10	-0.6853	-0.6804	-0.004
11	-0.6804	-0.6835	-0.004
12	-0.6835	-0.6815	-0.001
13	-0.6815	-0.6828	-0.001
14	-0.6828	**-0.6820**	**-0.0007**

Therefore, required root is **–0.682.**

Advantage: Economical and Easy Method

Disadvantage: No guarantee of convergence

1.9 REGULAR FALSI METHOD

Regular Falsi Method: The false-position method is a bracketing method similar to the bisection method laying the difference in the way that we obtain the new x_2 estimate. In this case the new x_2 is determined by $f(x_1)$ and $f(x_0)$. This method is also known as the *linear interpolation method* and as the formula:

$$x_2 = \frac{x_0 f(x_1) - x_1 f(x_0)}{f(x_1) - f(x_0)}$$

Example 1.3

Find a root of $3x + \sin x - e^x = 0$ using Regular Falsi Method.

Solution:

Now let us consider the function $f(x)$ in the interval [0, 0.5] where f (0) * f (0.5) is less than zero and use the Regular Falsi scheme to obtain the zero of $f(x) = 0$.

i.e., $x_0 = 0$

$x_1 = 0.5$

$$x_2 = \frac{x_0 f(x_1) - x_1 f(x_0)}{f(x_1) - f(x_0)} = 0.3757$$

N	x_0	x_1	x_2	$f(x_2)$
1	0.0000	0.5000	0.3757	0.0380
2 ($x_1 \leftarrow x_2$)	0.0000	0.3757	0.3619	0.0031
3 ($x_1 \leftarrow x_2$)	0.0000	0.3619	0.3605	0.0002
4 ($x_1 \leftarrow x_2$)	0.0000	0.3605	**0.3604**	**-0.0001**

Here $f(x_2)$ = -0.0001.

So one of the roots of $3x + \sin x - e^x = 0$ is approximately **0.3604**

Advantages:

1. Guaranteed convergence.

2. It will be superior to bisection method.

Disadvantages: It is; however, slow as it is first order convergent.

1.10 NEWTON RAPHSON METHOD

The Newton-Raphson Method: Methods such as bisection method and the false position method of finding roots of a nonlinear equation *f(x)=0* require bracketing of the root by two guesses. Such methods are called *bracketing* methods. These methods are always convergent since they are based on reducing the interval between the two guesses to *zero in* on the root.

In the Newton-Raphson method, the root is *not bracketed*. Only one initial guess of the root is needed to get the iterative process started to find the root of an equation. Hence, the method falls in the category of open methods. The Newton Raphson method is perhaps the most widely used of all root-locating formulas. Beside the initial guess, x_0, it's required that the first derivative, *f' (x),* is known. The converging this method is very fast. The Newton-Raphson formula:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

The sufficient condition for convergence of Newton-Raphson method is

$$\left| \frac{x_1 - x_0}{x_1} \right|.$$

Example 1.4

Solve the equation $f(x) = x^2 - 25 = 0$ using Newton-Raphson method.

Solution:

Given $\left|\frac{x_1 - x_0}{x_1}\right|$.

$f(x) = x^2 - 25 = 0$

$f'(x) = 2x$

Take $x_0 = 7$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 5.2857$$

The Iteration are

Iteration Number	***x_0***	***x_1***	***$f(x_0)$***	***$f(x_1)$***	$\left\|\frac{x_1 - x_0}{x_1}\right\|$
1	7	5.2857	24	14	.3242
2 ($x_0 \leftarrow x_1$)	5.2857	5.0070	2.9386	10.5714	.0527
3 ($x_0 \leftarrow x_1$)	5.0070	5.0000	0.0700	10.0140	.0013
4 ($x_0 \leftarrow x_1$)	5.0000	**5.0000**	0	10	**0**

Since $\left|\frac{x_1 - x_0}{x_1}\right| = 0$, when $x_1 = 0$.

Therefore, the root is **5.0000.**

Advantages:

1. It is rapidly convergent in most cases.

2. It is simple in its formulation, and therefore relatively easy to apply and program.

3. It is intuitive in its construction. This means it is easier to understand its behavior, when it is likely to behave well and when it may behave poorly.

Disadvantages:

1. It may not converge.

2. It needs to know both *f(x)* and *f′(x)*. Contrast this with the bisection method, which requires only *f (x)*.

1.11 SECANT METHOD

The Secant Method: The Secant Method is identical to the Newton-Raphson however the knowledge of the derivative is not needed, being this replaced by the backward finite divided difference. Note that this approach requires an additional initial estimate (x_{i-1}), resulting the formula:

$$x_{i+1} = \frac{x_i f(x_{i-1}) - x_{i-1} f(x_i)}{f(x_{i-1}) - f(x_i)}$$

Example 1.5

Find the root of the equation $e^x - 3x = 0$

Solution:

Given $f(x) = e^x - 3x = 0$

Let $x_0 = 1.5$ and $x_1 = 2$

$$x_2 = \frac{x_1 f(x_0) - x_0 f(x_1)}{f(x_0) - f(x_1)} = 1.5065$$

The iteration are

n	x_0	x_1	X_2	$f(x_2)$
1	1.5000	2	1.5065	-0.0085
2 $(x_0 \leftarrow x_2)$	1.5065	2	1.5090	-0.0047
3 $(x_0 \leftarrow x_2)$	1.5090	2	1.5106	-0.0023
4 $(x_0 \leftarrow x_2)$	1.5106	2	1.5113	-0.0012
5 $(x_0 \leftarrow x_2)$	1.5113	2	1.5116	-0.0008
6 $(x_0 \leftarrow x_2)$	1.5116	2	1.5118	-0.0005
7 $(x_0 \leftarrow x_2)$	1.5118	2	**1.5119**	**-0.0003**

Here $f\,(x_2)$ = -0.0003 when x_2 = 1.5119. Hence, the root is approximately **1.5119.**

Advantages:

1. It converges at faster than a linear rate, so that it is more rapidly convergent than the bisection method.
2. It does not require use of the derivative of the function, something that is not available in a number of applications.
3. It requires only one function evaluation per iteration, as compared with Newton's method, which requires two.

Disadvantages:

1. It may not converge.
2. There is no guaranteed error bound for the computed iterates.
3. Newton's method generalizes more easily to new methods for solving simultaneous systems of nonlinear equations.

1.12 CONVERGENCE CRITERIA OF ITERATIVE METHOD

The Convergence criteria of various iterative methods based on *order of convergence* and *evaluation of functions per iteration.*

S.No	Method	Formulae	Order of convergence	Evaluation of functions per iteration
1	Bisection	$x_2 = \frac{x_0 + x_1}{2}$	Gain of One per iteration	1
2	Fixed Point	$x_{n+1} = f(x_n)$	1	1
3	False Position	$x_2 = \frac{x_0 f(x_1) - x_1 f(x_0)}{f(x_1) - f(x_0)}$	1	1
4	Newton-Raphson	$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$	2	2
5	Secant	$x_{i+1} = \frac{x_i f(x_{i-1}) - x_{i-1} f(x_i)}{f(x_{i-1}) - f(x_i)}$	1.62	1

KEY WORDS

Keywords: Logic, Algorithm, Binary notation, Scientific notation, Associative, Distributive, Transcendental Function, Linear Interpolation method, Convergence, and Iteration.

LEARNING ACTIVITIES

a) Fill in the Blanks:

1) Non-linear equation is an equation containing a ________.

2) The new root estimate can be determined by ____________.

b) State whether true or False:

1) The Newton Raphson method is perhaps the most widely used of all root-locating formulas.

ANSWER TO LEARNING ACTIVITIES

a) Fill in the Blanks:

1) transcendental function

2) $x_2 = \frac{x_0 + x_1}{2}$

b) State whether true or False:

1) True

MODEL QUESTIONS:

1. Explain floating point numbers and its operations.
2. Discuss about the Non-Associativity of Arithmetic with example.
3. Write a note on Sources of Errors.
4. Write a note on Pitfalls in Computation.
5. What do you mean by Non-Linear equations?
6. Discuss about the Convergence Criteria of Iterative Method.
7. Find a real root correct to four decimals of the equation. $x^3 + 1.2x^2 - 4x - 4.8 = 0$ by Bisection Method.
8. Solve $3x - 1 - \cos x = 0$ by Fixed Point Method.
9. Solve $x^3 - 2x - 5 = 0$ by Regular Falsi Method.
10. Find a root of the equation $xe^x - 2 = 0$.
11. Solve $e^x - \sin x = 0$ using Secant Method.

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Block 2: Introduction

In this block, we will learn about the basic solution of linear algebraic equations. You will get clear idea about cramer's rule, gauss elimination rule, gauss Jordan, gauss seidal, jacobi's iterative method. This unit is divided into one unit are as follows.

Unit 2: it deals with solution of linear algebraic equations.

UNIT-2

SOLUTION OF LINEAR ALGEBRAIC EQUATIONS

Structure

Overview

Learning Objectives

2.1 System of Linear Equation

2.2 Cramer's Rule

2.3 Gauss Elimination Method

2.4 Pivoting Strategies

2.5 Gauss Jordan Method

2.6 Jacobi Iterative Method

2.7 Gauss Seidal Method

2.8 Comparison of Direct and Iterative Method

Keywords

Answer to Learning Activities

References

OVERVIEW

Many physical systems can be modeled by a set of linear equations which describe relationships between system variables. In simple cases, there are two or three variables; in complex systems (for example, in a linear model of the economy of a country) there may be several hundred variables. Linear systems also arise in connection with many problems of numerical analysis. Examples of these are the solution of partial differential equations by finite difference methods, statistical regression analysis, and the solution of eigen value problems.

Hence there arises a need for rapid and accurate methods for solving systems of linear equations. The student will already be familiar with solving by elimination systems of equations with two or three variables. This Step presents a formal description of the Gauss elimination method for *n*-variable systems.

LEARNING OBJECTIVES

After studying this unit, you should be able to discuss about

- System of linear equations
- Explain the concepts Cramer's Rule
- Discuss about the Pivoting Strategies
- To find solution of linear equation using Gauss Elimination, Jordan, Jacobi and Seidal Method
- Explain the concept of Diagonally Dominant
- Discuss Comparison of Direct and Iterative Method

2.1 SYSTEM OF LINEAR EQUATIONS

A linear equation in the *n* unknowns x_1, x_2, x_3 is an equation of the form:

$$a_1x_1 + a_2x_2 + \cdots + a_nx_n = b,$$

Where $a_1, a_2, \cdots a_n$ and *b* are constants.

The name *linear* comes from the fact that such an equation in two unknowns or variables represents a straight line. A set of such equations is called a *system*. An example of a system of three linear equations in the three unknowns *x*, *y* and *z* is:

$$\begin{cases} 4x + 8y + 4z = 80 \\ 2x + 1y - 4z = 7 \\ 3x - 1y + 2z = 22 \end{cases}$$

2.2 CRAMER'S RULE

Given a system of linear equations, Cramer's Rule is a handy way to solve for just one of the variables without having to solve the whole system of equations. They don't usually teach Cramer's Rule this way, but this is supposed to be the point of the Rule. Instead of solving the whole system, you can use Cramer's to solve for just one variable.

Cramer's Rule

Given the system of equation;

$a_1x + b_1y = c_1$

$a_2x + b_2y = c_2$ where the determinant

$$D = \begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix} \neq 0$$

Then,

$$X = \frac{\begin{vmatrix} c_1 & b_1 \\ c_2 & b_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} = \frac{D_x}{D}$$

and

$$y = \frac{\begin{vmatrix} a_1 & c_1 \\ a_2 & c_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}} = \frac{D_y}{D}$$

Example 2.1

Solve the system 7x – 5y = - 50 and 2x + y = - 7 using Cramer's Rule

Solution:

$$D = \begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix} = \begin{vmatrix} 7 & -5 \\ 2 & 1 \end{vmatrix} = 7 - (-10) = 17$$

$$D_x = \begin{vmatrix} b_1 & c_1 \\ b_2 & c_2 \end{vmatrix} = \begin{vmatrix} -5 & -50 \\ 1 & -7 \end{vmatrix} = 35 - (-50) = 85$$

$$D_y = \begin{vmatrix} a_1 & c_1 \\ a_2 & c_2 \end{vmatrix} = \begin{vmatrix} 7 & -50 \\ 2 & -7 \end{vmatrix} = -49 - (-100) = 51$$

$$x = \frac{D_x}{D} = \frac{85}{17} = 5 \qquad y = \frac{D_y}{D} = \frac{51}{17} = 3$$

Expanded Cramer's Rule

System of equation;

$a_1x + b_1y + c_1z = d_1$

$a_2x + b_2y + c_2z = d_2$

$a_3x + b_3y + c_3z = d_3$

where the determinant

$$D = \begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} \neq 0$$

Then,

$$D_x = \begin{vmatrix} d_1 & b_1 & c_1 \\ d_2 & b_2 & c_2 \\ d3 & b_3 & c_3 \end{vmatrix}$$

$$D_y = \begin{vmatrix} a_1 & d_1 & c_1 \\ a_2 & d_2 & c_2 \\ a3 & d_3 & c_3 \end{vmatrix}$$

$$D_z = \begin{vmatrix} a_1 & b_1 & d_1 \\ a_2 & b_2 & d_2 \\ a_3 & b_3 & d_3 \end{vmatrix}$$

and

$$x = \frac{D_x}{D}, y = \frac{D_y}{D} \,\&\, z = \frac{D_z}{D}$$

Example 2.2

Solve the following system of equations by Cramer's Rule:

$$5x - 2y + 3z = -1$$
$$3x + y - 2z = 25$$
$$2x - 4y + 5z = 16$$

Solution:

$$D = \begin{vmatrix} 5 & -2 & 3 \\ 3 & 1 & -2 \\ 2 & -4 & 5 \end{vmatrix} = 5\begin{vmatrix} 1 & -2 \\ -4 & 5 \end{vmatrix} -(-2)\begin{vmatrix} 3 & -2 \\ 2 & 5 \end{vmatrix} + 3\begin{vmatrix} 3 & 1 \\ 2 & -4 \end{vmatrix}$$

= 5(5-8) + 2(15-(-4)) + 3(-12 -2)

= 5(-3) + 2(19) + 3(-14)

= -15 + 38 - 42

= -19

D = -19

$$D_x = \begin{vmatrix} -1 & -2 & 3 \\ 25 & 1 & -2 \\ -29 & -4 & 5 \end{vmatrix} = -1\begin{vmatrix} 1 & -2 \\ -4 & 5 \end{vmatrix} -25\begin{vmatrix} -2 & 3 \\ -4 & 5 \end{vmatrix} - 29\begin{vmatrix} -2 & 3 \\ 1 & -2 \end{vmatrix}$$

= -1(5-8) -25(-10 - (-12)) - 29(4 - 3)

= -1(-3) -25(2) -29

= 3 - 50 -29

D_x= -76

$$D_y = \begin{vmatrix} 5 & -1 & 3 \\ 3 & 25 & -2 \\ 2 & -29 & 5 \end{vmatrix} = -(-1)\begin{vmatrix} 3 & -2 \\ 2 & 5 \end{vmatrix} + 25\begin{vmatrix} 5 & 3 \\ 2 & 5 \end{vmatrix} -(-29)\begin{vmatrix} 5 & 3 \\ 3 & -2 \end{vmatrix}$$

= 1(15 - (-4)) + 25 (25 -6) + 29 (-10 -9)

= 19 + 25(19) + 29(-19)

= 19(1 + 25 - 29)

= 19(-3)

D_y = -57

$$D_z = \begin{vmatrix} 5 & -2 & -1 \\ 3 & 1 & 25 \\ 2 & -4 & -29 \end{vmatrix} = -1 \begin{vmatrix} 3 & 1 \\ 2 & -4 \end{vmatrix} - 25 \begin{vmatrix} 5 & -2 \\ 2 & -4 \end{vmatrix} -29 \begin{vmatrix} 5 & -2 \\ 3 & 1 \end{vmatrix}$$

= -1(-12 - 2) -25(-20 - (-4)) - 29(5-(-6))

= -1(-14) -25(-16) -29(11)

= 14 + 400 - 319

= 95

$D_z = 95$

$$\therefore x = \frac{D_x}{D} = \frac{-76}{-19} = 4$$

$$y = \frac{D_y}{D} = \frac{-57}{-19} = 3$$

and

$$z = \frac{D_z}{D} = \frac{95}{-19} = -5$$

2.3 GAUSS ELIMINATION METHOD

Gaussian elimination is a method for solving matrix equations of the form $Ax = b$.

To perform Gaussian elimination starting with the system of equations

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} \\ a_{21} & a_{22} & \cdots & a_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{k1} & a_{k2} & \cdots & a_{kk} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_k \end{bmatrix},$$

Compose the "augmented matrix equation"

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1k} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2k} & b_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{k1} & a_{k2} & \cdots & a_{kk} & b_k \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix}.$$

Here, the column vector in the variables x is carried along for labeling the matrix rows. Now, perform elementary row operations to put the augmented matrix into the upper triangular form

$$\begin{bmatrix} a'_{11} & a'_{12} & \cdots & a'_{1k} & b'_1 \\ 0 & a'_{22} & \cdots & a'_{2k} & b'_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & a'_{kk} & b'_k \end{bmatrix}.$$

Solve the equation of the kth row for x_k, then substitute back into the equation of the $(k-1)$st row to obtain a solution for x_{k-1}, etc., according to the formula

$$x_i = \frac{1}{a'_{ii}}\left(b'_i - \sum_{j=i+1}^{k} a'_{ij}\, x_j\right).$$

A matrix that has undergone Gaussian elimination is said to be in echelon form.

Example 2.3

Solve the system of equations by Gauss Elimination method.

$x_1 + x_2 + x_3 = 3$

$2x_1 + 3x_2 + 7x_3 = 0$

$x_1 + 3x_2 - 2x_3 = 17$

Solution:

Consider the matrix equation

$$\begin{bmatrix} 1 & 1 & 1 \\ 2 & 3 & 7 \\ 1 & 3 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 0 \\ 17 \end{bmatrix}$$

In augmented form, this becomes

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 3 \\ 2 & 3 & 7 & 0 \\ 1 & 3 & -2 & 17 \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Subtracting the first from third row aand subtracting 2 times the first row from the second row gives

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 3 \\ 0 & 1 & 5 & -6 \\ 0 & 2 & -3 & 14 \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Subtracting 2 times the second row from the third row gives

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 3 \\ 0 & 1 & 5 & -6 \\ 0 & 0 & -13 & 26 \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Restoring the transformed matrix equation gives

$$\begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 5 \\ 0 & 0 & -13 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ -6 \\ 26 \end{bmatrix}$$

which can be solved immediately to give, $x_3 = 26/-13 = -2$ back-substituting to obtain $x_2 = 4$ and then again back-substituting to find $x_1 = 1$

2.4 PIVOTING STRATEGIES

A pivoting strategy is any procedure used to determine what to use for the diagonal entries as we apply row operations.

The diagonal entries that result from row operations as we move towards upper triangular form are referred to as pivots or pivot elements. We use row interchanges only to avoid zero pivots or small pivots. The reason for this is that pivots become denominators of the scalars in row operations as we move toward upper triangular form. Division by small values is a floating point arithmetic pitfall.

The selective use of row interchanges is referred to as a *PIVOTING STRATEGY.*

There are several common pivoting strategies:

• Natural order of pivots; no row interchanges permitted. With this strategy not every nonsingular linear system can be solved

• Row or Partial pivoting (also called Maximal column pivots)

• Scaled partial pivoting

• Full (complete) pivoting

Example 2.4

Solve the system of equations by Gauss Elimination method.

$9x_1 + 3x_2 + 4x_3 = 7$

$4x_1 + 3x_2 + 4x_3 = 8$

$x_1 + x_2 + x_3 = 3$

Solution:

Consider the matrix equation

$$\begin{bmatrix} 9 & 3 & 4 \\ 4 & 3 & 4 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 8 \\ 3 \end{bmatrix}$$

$$\begin{bmatrix} 9 & 3 & 4 & 7 \\ 4 & 3 & 4 & 8 \\ 1 & 1 & 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Interchange the first and third rows (without switching the elements in the right-hand column vector) gives

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 3 \\ 4 & 3 & 4 & 8 \\ 9 & 3 & 4 & 7 \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Subtracting 9 times the first row from the third row gives

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 3 \\ 4 & 3 & 4 & 8 \\ 0 & -6 & -5 & -20 \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Subtracting 4 times the first row from the second row gives

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 3 \\ 0 & -1 & 0 & -4 \\ 0 & -6 & -5 & -20 \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Finally, adding -6 times the second row to the third row gives

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 3 \\ 0 & -1 & 0 & -4 \\ 0 & 0 & -5 & 4 \end{array}\right]\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Restoring the transformed matrix equation gives

$$\begin{bmatrix} 1 & 1 & 1 \\ 0 & -1 & 0 \\ 0 & 0 & -5 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}=\begin{bmatrix} 3 \\ -4 \\ 4 \end{bmatrix}$$

Which can be solved immediately to give $x_3 = -4/5$,

Back-substituting to obtain $x_2 = 4$ and then again back-substituting to find $x_1 = -1/5$.

2.5 GAUSS JORDAN METHOD

This is a variation of Gaussian elimination. Gaussian elimination gives us tools to solve large linear systems numerically. It is done by manipulating the given matrix using the elementary row operations to put the matrix into row echelon form. To be in row echelon form, a matrix must conform to the following criteria:

1. If a row does not consist entirely of zeros, then the first non zero number in the row is a 1.(the leading 1)
2. If there are any rows entirely made up of zeros, then they are grouped at the bottom of the matrix.
3. In any two successive rows that do not consist entirely of zeros, the leading 1 in the lower row occurs farther to the right that the leading 1 in the higher row.

From this form, the solution is easily (relatively) derived. The variation made in the Gauss-Jordan method is called back substitution. Back substitution consists of taking a row echelon matrix and operating on it in reverse order. Normally the matrix is simplified from top to bottom to achieve row echelon form. When Gauss-Jordan has finished, all that remains in the matrix is a main diagonal of ones and the augmentation, this matrix is now in reduced row echelon form. For a matrix to be in reduced row echelon form, it must be in row echelon form and submit to one added criteria:

- Each column that contains a leading 1 has zeros everywhere else.

Since the matrix is representing the coefficients of the given variables in the system, the augmentation now represents the values of each of those variables. The solution to the system can now be found by inspection.

Example 2.5

Solve the system of equations by Gauss Jordan method.

$$\begin{aligned} 2x_1 + x_2 - x_3 &= -2 \\ x_2 + 2x_3 &= 2 \\ x_1 - x_2 + x_3 &= 5 \end{aligned}$$

Solution:

Consider the matrix equation

$$\begin{bmatrix} 2 & 1 & -1 \\ 0 & 1 & 2 \\ 1 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -2 \\ 2 \\ 5 \end{bmatrix}$$

In augmented form, this becomes

$$\begin{bmatrix} 2 & 1 & -1 & -2 \\ 0 & 1 & 2 & 2 \\ 1 & -1 & 1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Interchange the first and third rows gives

$$\begin{bmatrix} 1 & -1 & 1 & 5 \\ 0 & 1 & 2 & 2 \\ 2 & 1 & -1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Subtracting 2 times the first row from the third row gives

$$\begin{bmatrix} 1 & -1 & 1 & 5 \\ 0 & 1 & 2 & 2 \\ 0 & 3 & -3 & -12 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Add second row with first row gives

$$\begin{bmatrix} 1 & 0 & 3 & 7 \\ 0 & 1 & 2 & 2 \\ 0 & 3 & -3 & -12 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Subtracting 3 times the second row from the third row gives

$$\begin{bmatrix} 1 & 0 & 3 & 7 \\ 0 & 1 & 2 & 2 \\ 0 & 0 & -9 & -18 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Divide the third row by 9 then,

$$\begin{bmatrix} 1 & 0 & 3 & 7 \\ 0 & 1 & 2 & 2 \\ 0 & 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Subtracting 2 times the third row from the second row gives,

$$\begin{bmatrix} 1 & 0 & 3 & 7 \\ 0 & 1 & 0 & -2 \\ 0 & 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Subtracting 3 times the third row from the first row gives,

$$\begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & -2 \\ 0 & 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$\Rightarrow x_1 = 1, x_2 = -2, x_3 = 2$

2.6 JACOBI ITERATIVE METHOD

Diagonally Dominant: Simpler test of convergence is that if the matrix A is strictly diagonally dominant then the iterations will converge.

Matrix A is strictly diagonally dominant if the diagonal element of a row (in absolute terms) is greater than the sum of all the other terms in the row.

Example

$$ie., |a_{ii}| > \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{ij}|; i$$

$$\begin{bmatrix} 10 & 3 & -1 \\ -3 & 10 & 2 \\ 1 & 2 & 10 \end{bmatrix}$$

So matrix is strictly diagonally dominant.

Jacobi and Seidal iterations using this matrix will converge.

Jacobi Iteration Method: The Jacobi method is easily derived by examining each of the n equations in the linear system n. If in the i^{th} equation

$$\sum_{j=1}^{n} a_{i,j} x_j = b$$

we solve for the value of x_i while assuming the other entries of x remain fixed, we obtain

$$x_i = \frac{1}{a_{i,j}}(b_i - \sum_{j \neq i} a_{i,j} x_j),$$

This suggests an iterative method defined by

$$x_i^{(k)} = \frac{1}{a_{i,j}}(b_i - \sum_{j \neq i} a_{i,j} x_j^{(k-1)}),$$

which is the Jacobi method. Note that the order in which the equations are examined is irrelevant, since the Jacobi method treats them independently. For this reason, the Jacobi method is also known as the *method of simultaneous displacements*, since the updates could in principle be done simultaneously.

Now to find x_i's, assumes an initial values for the x_i's are zero in Jacobi Iteration Method.

Example 2.6

Given the system of equations,

$$10x_1 + x_2 + x_3 = 12$$

$$x_1 + x_2 + 10x_3 = 12$$

$$x_1 + 10x_2 + x_3 = 12.$$

Find the solution using Gauss Jacobi Iteration Method.

Solution:

The coefficient matrix

$$[A]=\begin{bmatrix}10 & 1 & 1\\ 1 & 1 & 10\\ 1 & 10 & 1\end{bmatrix}.$$

We note that A is not diagonally dominant.

However it can be made diagonally dominant by changing the rows as

$$[A]=\begin{bmatrix}10 & 1 & 1\\ 1 & 10 & 1\\ 1 & 1 & 10\end{bmatrix}$$

Rewriting the equations, we get

$$x_1=\frac{12-x_2-x_3}{10}$$

$$x_2=\frac{12-x_1-x_3}{10}$$

$$x_3=\frac{12-x_1-x_2}{10}$$

Assuming an initial guess of

$$\begin{bmatrix}x_1\\ x_2\\ x_3\end{bmatrix}=\begin{bmatrix}0\\ 0\\ 0\end{bmatrix}$$

<u>Iteration 1:</u>

$$x_1=\frac{12-0-0}{10}$$

$$=1.2000$$

$$x_2=\frac{12-0-0}{10}$$

$$=1.2000$$

Iteration 2:

$$x_1 = \frac{12-1.2-1.2}{10} = 0.96$$

$$x_2 = \frac{12-1.2-1.2}{10} = 0.96$$

$$x_3 = \frac{12-1.2-1.2}{10} = 0.96$$

The above iterations can be simply carried out exhibited in the following tabular form

Iteration	$x_1 = \frac{12-x_2-x_3}{10}$	$x_2 = \frac{12-x_1-x_3}{10}$	$x_3 = \frac{12-x_1-x_2}{10}$
1	1.2000	1.2000	1.2000
2	0.9600	0.9600	0.9600
3	1.0080	1.0080	1.0080
4	0.9984	0.9984	0.9984
5	1.0003	1.0003	1.0003
6	0.9999	0.9999	0.9999
7	1.0000	1.0000	1.0000
8	1.0000	1.0000	1.0000

This is close to the exact solution vector of

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

2.7 SIEDAL ITERATIVE METHOD

Gauss Seidal Method: Given a general set of *n* equations and *n* unknowns, we have

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = c_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2n}x_n = c_2$$

$$\vdots \qquad \vdots$$

$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \ldots + a_{nn}x_n = c_n$$

If the diagonal elements are non-zero, each equation is rewritten for the corresponding unknown, that is, the first equation is rewritten with x_1 on the left hand side and the second equation is rewritten with x_2 on the left hand side and so on as follows

$$x_1 = \frac{c_1 - a_{12}x_2 - a_{13}x_3 \ldots\ldots - a_{1n}x_n}{a_{11}}$$

$$x_2 = \frac{c_2 - a_{21}x_1 - a_{23}x_3 \ldots\ldots - a_{2n}x_n}{a_{22}}$$

$$\vdots$$

$$\vdots$$

$$x_{n-1} = \frac{c_{n-1} - a_{n-1,1}x_1 - a_{n-1,2}x_2 \ldots\ldots - a_{n-1,n-2}x_{n-2} - a_{n-1,n}x_n}{a_{n-1,n-1}}$$

$$x_n = \frac{c_n - a_{n1}x_1 - a_{n2}x_2 - \ldots\ldots - a_{n,n-1}x_{n-1}}{a_{nn}}$$

These equations can be rewritten in the summation form as

$$x_1 = \frac{c_1 - \sum_{\substack{j=1 \\ j\neq 1}}^{n} a_{1j}x_j}{a_{11}}$$

$$x_2 = \frac{c_2 - \sum_{\substack{j=1 \\ j \neq 2}}^{n} a_{2j} x_j}{a_{22}}$$

.

.

.

$$x_{n-1} = \frac{c_{n-1} - \sum_{\substack{j=1 \\ j \neq n-1}}^{n} a_{n-1,j} x_j}{a_{n-1,n-1}}$$

$$x_n = \frac{c_n - \sum_{\substack{j=1 \\ j \neq n}}^{n} a_{nj} x_j}{a_{nn}}$$

Hence for any row *i*,

$$x_i = \frac{c_i - \sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij} x_j}{a_{ii}}, i = 1,2,\ldots,n.$$

Now to find x_i's, one assumes an initial guess for the x_i's and then use the rewritten equations to calculate the new guesses.

Example 2.7

Given the system of equations,

$$12x_1 + 3x_2 - 5x_3 = 1$$

$$3x_1 + 7x_2 + 13x_3 = 76$$

$$x_1 + 5x_2 + 3x_3 = 28.$$

Find the solution using Gauss Seidal Method.

Solution:

The coefficient matrix

$$[A]=\begin{bmatrix}12 & 3 & -5\\ 3 & 7 & 13\\ 1 & 5 & 3\end{bmatrix}.$$

We note that A is not diagonally dominant.

However it can be made diagonally dominant by changing the rows as

$$[A]=\begin{bmatrix}12 & 3 & -5\\ 1 & 5 & 3\\ 3 & 7 & 13\end{bmatrix}$$

Rewriting the equations, we get

$$x_1=\frac{1-3x_2+5x_3}{12}$$

$$x_2=\frac{28-x_1-3x_3}{5}$$

$$x_3=\frac{76-3x_1-7x_2}{13}$$

Assuming an initial guess of

$$\begin{bmatrix}x_1\\ x_2\\ x_3\end{bmatrix}=\begin{bmatrix}1\\ 0\\ 1\end{bmatrix}$$

<u>Iteration 1:</u>

$$x_1=\frac{1-3(0)+5(1)}{12}\quad=\quad 0.50000$$

$$x_2=\frac{28-(0.5)-3(1)}{5}\quad=\quad 4.9000$$

$$x_3 = \frac{76 - 3(0.50000) - 7(4.9000)}{13} \quad = \quad 3.0923$$

Iteration 2:

$$x_1 = \frac{1 - 3(4.9000) + 5(3.0923)}{12} \quad = \quad 0.14679$$

$$x_2 = \frac{28 - (0.14679) - 3(3.0923)}{5} \quad = \quad 3.7153$$

$$x_3 = \frac{76 - 3(0.14679) - 7(4.900)}{13} \quad = \quad 3.8118$$

The above iterations can be simply carried out exhibited in the following tabular form

Iteration	$x_1 = \frac{1 - 3x_2 + 5x_3}{12}$	$x_2 = \frac{28 - x_1 - 3x_3}{5}$	$x_3 = \frac{76 - 3x_1 - 7x_2}{13}$
1	0.50000	4.900	3.0923
2	0.14679	3.7153	3.8118
3	0.74275	3.1644	3.9708
4	0.94675	3.0281	3.9971
5	0.99177	3.0034	4.0001
6	0.99919	3.0001	4.0001

This is close to the exact solution vector of

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \\ 4 \end{bmatrix}$$

2.8 COMPARISON OF DIRECT AND ITERATIVE METHODS

Both direct and iterative method has their strengths and weakness and a choice is based on the particular set of equations to be solved.

Direct Method	**Iterative Method**
The computational effort is approximately ($2n^3/3$) arithmetic operations in each step.	Computational effort is approximately ($2n^2$) arithmetic operations per iteration.
The rounding errors may become quite large.	Iterative method is the small rounding error.
Any special structure in the matrix of coefficients is difficult to preserve during elimination	Special pattern of zeros in the coefficient matrix could be used to tailor a procedure with reduced calculation effort.

KEY WORDS

Keywords: Linear Equation, Matrix, Echelon form, Diagonal, Pivot, Diagonally dominant, Simultaneous Displacement, Coefficient.

LEARNING ACTIVITIES

a) Fill in the blanks:

1) The Jacobi method is also known as the____________..

b) State whether true or False:

1) The variation made in the Gauss-Jordan method is called back substitution

Answer to learning Activities

a) Fill in the blanks:

1) *Method of simultaneous displacements*

b) Sta te whether true or False:

1) True

Model Questions

1. Solve the following system of equations by Cramer's Rule

$$x+2y+3z=10$$
$$2x-3y+z=1$$
$$3x+y-2z=9$$

2. Solve using Cramer's Rule

$$x_1+x_2+x_3=6$$
$$x_1-x_2+x_3=2$$
$$2x_1+x_2-x_3=1$$

3. Solve the following system of equations by Gauss Elimination Method

$$x_1-x_2+x_3=1$$
$$-3x_1+2x_2-3x_3=-6$$
$$2x_1-5x_2+4x_3=5$$

4. Solve the following system of equations by Gauss Jordan Method

$$10x_1+x_2+x_3=12$$
$$2x_1+10x_2+x_3=13$$
$$x_1+x_2+5x_3=7$$

5. Solve the following system of equations by Jacobi Method

$$x_1+17x_2-2x_3=48$$
$$x_1+x_2+9x_3=30$$
$$30x_1-2x_2+3x_3=48$$

6. Given the system of equations

$$3x_1 + 7x_2 + 13x_3 = 76$$

$$x_1 + 5x_2 + 3x_3 = 28$$

$$12x_1 + 3x_2 - 5x_3 = 1$$

find the solution using Gauss-Seidal method.

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Block 3: Introduction

In this block, we will learn about the basic of interpolation and curve fitting. We will get a clear idea about langranges method, Newton's interpolation, least Square approximation etc... this block is divided into one unit are as follows

Unit 3: It deals with interpolation and Curve Fitting.

UNIT-3

INTERPOLATION AND CURVE FITTING

Structure

Overview

Learning Objectives

3.1 Problem of Interpolation

3.2 Lagranges method of Interpolation

3.3 Inverse Interpolation

3.4 Newton's Interpolation Formulae

3.5 Interpolation at Equally spaced points of Newton's Forward and backward difference formulae

3.6 Error of the Interpolating Polynomial

3.7 Fitting of polynomials and Curve

3.8 Least square approximation of functions

3.9 Linear and Polynomial Regression

Keywords

Answer to Learning Activities

References

OVERVIEW

In engineering applications, data collected from the field are usually discrete and the physical meanings of the data are not always well known. To estimate the outcomes and, eventually, to have a better understanding of the physical phenomenon, a more analytically controllable function that fits the field data is desirable. The process of finding the coefficients for the fitting function is called *curve fitting*; the process of estimating the outcomes in between sampled data points is called *interpolation*; whereas the process of estimating the outcomes beyond the range covered by the existing data is called *extrapolation*.

LEARNING OBJECTIVES

After studying this unit, you should be able to discuss about

- Numerical Interpolation concept
- To explain Lagrange's Interpolation Method
- Discuss Euler's Method, Improved Euler's Method and Modified Euler's Method

3.1 PROBLEM OF INTERPOLATION

In the mathematical subfield of numerical analysis, *interpolation* is a method of constructing new data points from a discrete set of known data points.

A different problem which is closely related to interpolation is the approximation of a complicated function by a simple function. Suppose we know the function but it is too complex to evaluate efficiently. Of course, when using the simple function to calculate new data points we usually do not receive the same result as when using the original function, but depending on the problem domain and the interpolation method used the gain in simplicity might offset the error.

3.2 LAGRANGE'S METHOD OF INTERPOLATION

Many a times, a function $y = f(x)$ is given only at discrete points such as $(x_0, y_0), (x_1, y_1), \ldots\ldots, (x_{n-1}, y_{n-1}), (x_n, y_n)$. How does one find the value of 'y' at any other value of 'x'? Well, a continuous function $f(x)$ may be used to represent the 'n+1' data values with $f(x)$ passing through the 'n+1' points. Then one can find the value of y at any other value of x. This is called interpolation. Of course, if 'x' falls outside the range of 'x' for which the data is given, it is no longer interpolation but instead is called extrapolation.

Since Lagrange's interpolation is also an Nth degree polynomial approximation to f(x) and the Nth degree polynomial passing through (N+1) points is unique. However, Lagrange's formula is more convenient to use in computer programming.

Polynomial interpolation involves finding a polynomial of order 'n' that passes through the 'n+1' points. One of the methods to find this polynomial is called Lagrangian Interpolation. Other methods include the direct method and the Newton's Divided Difference Polynomial method.

Lagrangian interpolating polynomial is given by

$$f_n(x) = \sum_{i=0}^{n} L_i(x) f(x_i)$$

where 'n' in $f_n(x)$ stands for the n^{th} order polynomial that approximates the function $y = f(x)$ given at $(n+1)$ data points as $(x_0, y_0), (x_1, y_1), \ldots\ldots, (x_{n-1}, y_{n-1}), (x_n, y_n)$, and

$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

$L_i(x)$ is a weighting function that includes a product of $(n-1)$ terms with terms of $j = i$ omitted.

Hence Lagrange's Interpolation formula is,

$$f(x) = \frac{(x-x_1)(x-x_2)\cdots(x-x_n)}{(x_0-x_1)(x_0-x_2)\cdots(x_0-x_n)} f(x_0) + \frac{(x-x_0)(x-x_2)\cdots(x-x_n)}{(x_1-x_0)(x_1-x_2)\cdots(x_1-x_n)} f(x_0) +$$

$$+ \cdots + \frac{(x-x_0)(x-x_1)\cdots(x-x_{n-1})}{(x_n-x_0)(x_n-x_1)\cdots(x_n-x_{n-1})} f(x_n)$$

Example 3.1

Using Lagrange's formula find the value of y when x = 0.3. The values of x and y are:

x	**0**	**1**	**3**	**4**	**7**
y	**1**	**3**	**49**	**129**	**813**

Solution:

Here $x_0 = 0$, $x_1 = 1$, $x_2 = 3$ $x_3 = 4$, $x_4 = 7$ and $x = 0.3$

By Lagrange's Interpolation formula,

$$f(x) = \frac{(x-x_1)(x-x_2)(x-x_3)(x-x_4)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)(x_0-x_4)} f(x_0) + \frac{(x-x_0)(x-x_2)(x-x_3)(x-x_4)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)(x_1-x_4)} f(x_1) +$$

$$+\cdots+ \frac{(x-x_0)(x-x_1)(x-x_2)(x-x_3)}{(x_4-x_0)(x_4-x_1)(x_4-x_2)(x_4-x_3)} f(x_4)$$

$$= \frac{(0.3-1)(0.3-3)(0.3-4)(0.3-7)}{(-1)(-3)(-4)(-7)} 1$$

$$+ \frac{(0.3-0)(0.3-3)(0.3-4)(0.3-7)}{(1)(-2)(-3)(-6)} 3$$

$$+ \frac{(0.3-0)(0.3-1)(0.3-4)(0.3-7)}{(3)(2)(-1)(-4)} 49$$

$$+ \frac{(0.3-0)(0.3-1)(0.3-3)(0.3-7)}{(4)(3)(1)(-3)} 129$$

$$+ \frac{(0.3-0)(0.3-1)(0.3-3)(0.3-4)}{(7)(6)(4)(3)} 813$$

= 1.831

3.3 INVERSE INTERPOLATION

Inverse Interpolation is defined as the process of calculating the value of argument corresponding to a given value lying between two tabulated functional values.

In the Lagrange's interpolation formula, we have treated y as the dependent variable that was expressed as a function of the independent variable x. If we treat x as function y as independent variable then Lagrange's Interpolation formula can be put as

$$x=\frac{(y-y_1)(y-y_2)\cdots(y-y_n)}{(y_0-y_1)(y_0-y_2)\cdots(y_0-y_n)}x_0+\frac{(y-y_0)(y-y_2)\cdots(y-y_n)}{(y_1-y_0)(y_1-y_2)\cdots(y_1-y_n)}x_1+$$

$$+\cdots+\frac{(y-y_0)(y-y_1)\cdots(y-y_{n-1})}{(y_n-y_0)(y_n-y_1)\cdots(y_n-y_{n-1})}x_n$$

Example 3.2

Using Lagrange's Inverse Interpolation formula find the value of x when y = 19. The values of x and y are:

Y	0	1	20
X	0	1	2

Solution:

Here $x_0 = 0$, $x_1 = 1$, $x_2 = 2$, $y_0=0$, $y_1=1$, and $y_2=20$

By Lagrange's Interpolation formula,

$$x=\frac{(y-y_1)(y-y_2)}{(y_0-y_1)(y_0-y_2)}x_0+\frac{(y-y_0)(y-y_2)}{(y-y)(y-y)}x_1+\frac{(y-y_0)(y-y_1)}{(y_2-y_0)(y_2-y_1)}x_2$$

$$=\frac{(19-1)(19-20)}{(0-1)(0-20)}0+\frac{(19-0)(19-20)}{(1-0)(1-20)}1+\frac{(19-0)(19-1)}{(20-0)(20-1)}2$$

$$=0+1+1.8$$

$$=2.8$$

Let the function *f* be tabulated at the (not necessarily equidistant) points $[x_0, x_1, \ldots, x_n]$. We define the *divided differences* between points as follows:

first divided and difference between x_0 and x_1 by,

$$f(x_0, x_1) = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

and it is denoted by $\Delta f(x_0)$.

Similarly,

$$\Delta f(x_1) = f(x_1, x_2) = \frac{f(x_2) - f(x_1)}{x_2 - x_1}$$

$$\vdots$$

$$\Delta f(x_{n-1}) = f(x_{n-1}, x_n) = \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

Second divided and difference between x, x_0, x_1 by,

$$\Delta^2 f(x_0) = f(x_0, x_1, x_2) = \frac{f(x_1, x_2) - f(x_0, x_1)}{x_2 - x_0}$$

Similarly, the nth divided differences is given by,

$$\Delta^n f(x_0) = f(x_0, x_1, \ldots, x_{n-1}) = \frac{f(x_1, x_2, \ldots, x_n) - f(x_0, x_1, \ldots, x_{n-1})}{x_n - x_0}$$

The divided differences are conveniently evaluated within a table, shown in symbolic form in Table. Notice that the table is arranged so that the function values required at each stage are adjacent.

Table: Divided Difference Table

i	x_i	$f(x_i)$				
0	x_0	$f(x_0)$				
			$f[x_0, x_1]$			
1	x_1	$f(x_1)$		$f[x_0, x_1, x_2]$		
			$f[x_1, x_2]$		$f[x_0, x_1, x_2, x_3]$	
2	x_2	$f(x_2)$		$f[x_1, x_2, x_3]$		$f[x_0, x_1, x_2, x_3, x_4]$
			$f[x_2, x_3]$		$f[x_1, x_2, x_3, x_4]$	
3	x_3	$f(x_3)$		$f[x_2, x_3, x_4]$		
			$f[x_3, x_4]$			
4	x_4	$f(x_4)$				

Example 3.3

Construct the Divided Difference for the following data:

x	0	1	3	6	10
$f(x)$	1	-6	4	169	921

Solution:

The divided difference Table:

x	$f(x)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$	$\Delta^4 f(x)$
0	1				
		-7			
1	-6		4		
		5		1	
3	4		10		0
		55		1	
6	169		19		
		188			
10	921				

3.4 NEWTON'S INTERPOLATION FORMULAE

According to divided differences, we find

$$f(x) = f(x_0) + (x - x_0) f(x, x_0)$$

$$f(x, x_0) = f(x_0, x_1) + (x - x_1) f(x, x_0, x_1)$$

$$f(x, x_0, x_1) = f(x_0, x_1, x_2) + (x - x_2) f(x, x_0, x_1, x_2)$$

$$\vdots \qquad \vdots \qquad \vdots \qquad \vdots$$

$$f(x, x_0, \ldots, x_{n-1}) = f(x_0, x_1, \ldots x_n) + (x - x_n) f(x, x_0, \ldots, x_n)$$

i.e. Multiplying the second equation by $(x-x_0)$, the third by $(x-x_0)(x-x_1)$. etc., and adding the results yields Newton's divided difference formula,

$$f(x) = f(x_0) + (x - x_0) f(x_0, x_1) + (x - x_0)(x - x_1) f(x_0, x_1, x_2)$$

$$+ \cdots + (x - x_0) \cdots (x - x_{n-1}) f(x_0, x_1, \ldots, x_n) + R$$

where $R=(x-x_0)(x-x_1)\cdots(x-x_n)f(x,x_0,x_1,\ldots x_n)$.

The remainder term R vanishes at x_0, $x_1,\ldots$, x_n, where we infer that the other terms on the right-hand side constitute the interpolating polynomial or, equivalently, the Lagrange polynomial. If the required degree of the interpolating polynomial is not known in advance, it is customary to arrange the points x_1, … , x_n, according to their increasing distance from x and add terms until *R* is small enough.

Example 3.4

Given

x	0	0.2	0.4
$f(x)$	0	0.198669	0.389418

find $f(0.1)$ using Newton's Interpolation formula.

Solution:

The divided difference Table:

x	$F(x)$	$\Delta f(x)$	$\Delta^2 f(x)$
0	0		
		0.993345	
0.2	0.198669		-0.099000
		0.953745	
0.4	0.389418		

Using Newton's Interpolation formula, we get,

$$f(x)=f(x_0)+(x-x_0)f(x_0,x_1)+(x-x_0)(x-x_1)f(x_0,x_1,x_2)+\cdots$$

$$f(0.1)=0+(0.1-0)\times 0.993345+(0.1-0)\times(0.1-0.2)\times(-0.099000)$$

$$=0.100325.$$

3.5 INTERPOLATION AT EQUALLY SPACED POINTS

Lagrange Interpolation has a number of disadvantages

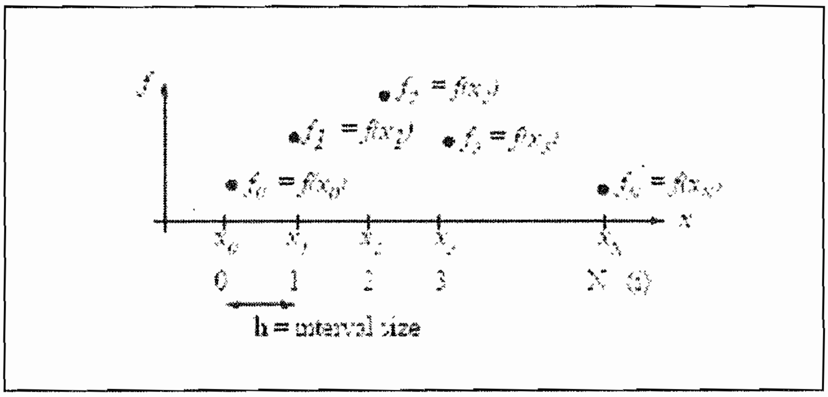
- The amount of computation required is large
- Interpolation for additional values of requires the same amount of effort as the first value (i.e. no part of the previous calculation can be used)
- When the number of interpolation points are changed (increased/ decreased), the results of the previous computations can not be used
- Error estimation is difficult (at least may not be convenient)

Use Newton Interpolation which is based on developing difference tables for a given set of data points

- The N-th degree interpolating polynomial obtained by fitting N+1 data points will be identical to that obtained using Lagrange formulae!
- Newton interpolation is simply *another* technique for obtaining the same interpolating polynomial as was obtained using the Lagrange formulae.

Newton's Forward Difference Formula:

We assume equi-spaced points



Forward differences are now defined as follows:

We take $x_i = x_0 + ih, \ i = 0,1,....,$ where h is the interval width. The divided differences can be simplified, since we no longer need to show the interval width explicitly. For this case we define the *forward difference* by

$$\Delta f(x) = f(x+h) - f(x) \text{ or } \Delta f(x_i) = f(x_{i+1}) - f(x_i).$$

The connection between this and the equivalent divided difference is given by

$$f(x_0, x_1) = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{\Delta f(x_0)}{h},$$

$$\text{or } \Delta f(x_0) = hf(x_0, x_1).$$

We now regard Δ as the forward difference operator, which operates on $f(x_i)$ to give $f(x_{i+1}) - f(x_i)$. Thus

$$\begin{aligned} \Delta^2 f(x_i) &= \Delta(\Delta f(x_i)) \\ &= \Delta(f(x_{i+1}) - f(x_i)) \\ &= f(x_{i+2}) - f(x_{i+1}) - (f(x_{i+1}) - f(x_i)) \\ &= f(x_{i+2}) - 2f(x_{i+1}) + f(x_i). \end{aligned}$$

It is easy to check that Δ is linear operator, that is, it satisfies

$$\Delta(\lambda f(x) + \mu g(x)) = \lambda \Delta f(x) + \mu \Delta g(x)$$

Which allows simpler manipulations.

Proceeding slightly differently, we obtain

$$\begin{aligned} \Delta^2 f(x_i) &= f(x_{i+2}) - f(x_{i+1}) - (f(x_{i+1}) - f(x_i)) \\ &= hf[x_{i+1}, x_{i+2}] - hf[x_i, x_{i+1}] \\ &= h^2 f[x_i, x_{i+1}, x_{i+2}]. \end{aligned}$$

You will use induction in an exercise to prove the results

$$\begin{aligned} \Delta^n f(x_i) &= \textstyle\sum_{k=0}^{n} (-1)^{n-k} \binom{n}{k} f(x_{i+k}) \\ &= n! h^n f[x_i, x_{i+1}, \ldots, x_{i+n}] \\ &= h^n f^{(n)}(\xi), \quad x_i < \xi < x_{i+n}. \end{aligned}$$

Newton's divided Difference Interpolating Polynomial now becomes

$$y = f(x_0) + (x - x_0) f(x_0, x_1) + (x - x_0)(x - x_1) f(x_0, x_1, x_2) + \cdots$$

$$\ldots \; + (x - x_0)(x - x_1) \cdots (x - x_n) f(x_0, x_1, \ldots, x_n)$$

$$= f(x_0) + sh \frac{\Delta f(x_0)}{h} + sh(sh - h) \frac{\Delta^2 f(x_0)}{h^2 2!} + \cdots + sh(sh-1) \cdots (sh - (n-1)h) \frac{\Delta^n f(x_0)}{h^n n!}$$

$$= f(x_0) + s \Delta f(x_0) + \frac{s(s-1)}{2!} \Delta^2 f(x_0) + \cdots + \frac{s(s-1) \cdots (s-n+1)}{n!} \Delta^n f(x_0)$$

where $s = \dfrac{x - x_0}{h}$.

The forward differences are computed in a tabular form similar to that for divided differences. Typically we set up a difference table.

i	f_i	Δf_i	$\Delta^2 f_i$	$\Delta^3 f_i$	$\Delta^4 f_i$
0	f_0	$\Delta f_0 = f_1 - f_0$	$\Delta^2 f_0 = \Delta f_1 - \Delta f_0$	$\Delta^3 f_0 = \Delta^2 f_1 - \Delta^2 f_0$	$\Delta^4 f_0 = \Delta^3 f_1 - \Delta^3 f_0$
1	f_1	$\Delta f_1 = f_2 - f_1$	$\Delta^2 f_1 = \Delta f_2 - \Delta f_1$	$\Delta^3 f_1 = \Delta^2 f_2 - \Delta^2 f_1$	
2	f_2	$\Delta f_2 = f_3 - f_2$	$\Delta^2 f_2 = \Delta f_3 - \Delta f_2$		
3	f_3	$\Delta f_3 = f_4 - f_3$			
4	f_4				

Newton's Backward Difference Formula:

There is also a *backward difference operator*, ∇, which is defined by

$$\nabla f(x) = f(x) - f(x - h),$$

Hence we have Newton's Backward formula for equal intervals is,

$$y = f(x_n) + \frac{s}{1!} \nabla f(x_n) + \frac{s(s+1)}{2!} \nabla^2 f(x_n) \cdots + \frac{s(s+1) \cdots (s+n-1)}{n!} \nabla^n f(x_n).$$

Where $s = \dfrac{x - x_n}{h}$.

Example 3.5

Given

X	0	2	4	6
$F(x)$	2	0	2	20

find $f(5)$ using Newton's Forward Difference formula.

Solution:

The Difference table is:

x	$f(x)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$
0	2			
		-2		
2	0		4	
		2		12
4	2		16	
		18		
6	20			

Here $x_0 = 0$, x = 4 and h = 2.

By Newton's Forward Difference Formula,

$$= f(x_0) + s\Delta f(x_0) + \frac{s(s-1)}{2!}\Delta^2 f(x_0) + \cdots + \frac{s(s-1)\cdots(s-n+1)}{n!}\Delta^n f(x_0)$$

where $s = \dfrac{x - x_0}{h}$.

Hence $s = \dfrac{5-0}{2} = 2.5$

$$\text{Hence y} = 2 + \frac{(2.5)}{1}(-2) + \frac{2.5\times1.5}{2}4 + \frac{2.5\times1.5\times.5}{6}12$$

$$= 2 - 5 + 7.5 + 3.75$$

$$= 8.25$$

Example 3.6

Given

x	1961	1971	1981	1991	2001
y	46	66	81	93	101

find $f(1996)$ using Newton's Forward Difference formula.

Solution:

X	Y	∇y	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$
1961	46				
		20			
1971	66		- 5		
		15		2	
1981	81		- 3		- 3
		12		- 1	
1991	93		- 4		
		8			
2001	101				

By Newton's Backward Interpolation formula,

$$y = f(x_n) + \frac{s}{1!}\nabla f(x_n) + \frac{s(s+1)}{2!}\nabla^2 f(x_n)\cdots + \frac{s(s+1)\cdots(s+n-1)}{n!}\nabla^n f(x_n).$$

Where $s = \dfrac{x - x_n}{h}$.

Here x = 1996, x_n = 2001 and h = 10

Hence $s = \dfrac{x - x_n}{h} = \dfrac{1996 - 2001}{10} = -0.5$

Hence,

$$y = 101 + \frac{-0.5}{1}8 + \frac{(-0.5)(0.5)}{2}(-4) + \frac{(-0.5)(0.5)(1.5)}{6}(-1) + \frac{(-0.5)(0.5)(1.5)(2.5)}{24}(-3)$$

$$= 101 - 4 + 0.5 + 0.0625 + 0.1171875$$

$$= 97.6796875$$

3.6 ERROR OF THE INTERPOLATING POLYNOMIALS

Suppose that the interpolation polynomial is in the form

$$p(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_2 x^2 + a_1 x + a_0.$$

The statement that p interpolates the data points means that

$$p(x_i) = y_i \qquad \text{for all } i \in \{0, 1, \ldots, n\}.$$

When interpolating a given function *f* by a polynomial of degree *n* at the nodes $x_0,\ldots,x_n$ we get the error

$$f(x) - p_n(x) = f[x_0, \ldots, x_n, x] \prod_{i=0}^{n} (x - x_i)$$

where $f[x_0, \ldots, x_n, x]$ is the notation for divided differences. When *f* is *n*+1 times continuously differentiable on the smallest interval *I* which contains the nodes x_i and *x* then we can write the error in the Lagrange form as

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x - x_i)$$

for some ξ in *I*. Thus the remainder term in the Lagrange form of the Taylor theorem is a special case of interpolation error when all interpolation nodes x_i are identical.

In the case of equally spaced interpolation nodes $x_i = x_0 + ih$, it follows that the interpolation error is $O(h^n)$. However, this does not necessarily mean that the error goes to zero as $n \to \infty$. In fact, the error may increase without bound near the ends of the interval $[x_0,x_n]$. This is called Runge's phenomenon.

The above error bound suggests choosing the interpolation points x_i such that the product $|\prod (x - x_i)|$ is as small as possible.

Newton's Interpolation Error:

Assume that $f(x)$ defined on $[a, b]$, which contains the equally spaced nodes $x_k = x_0 + kh$. Additionally, assume that $f(x)$ and the derivatives of $f(x)$ up to the order $n+1$ are continuous and bounded on the special subintervals $[x_0, x_1]$, $[x_0, x_2]$, $[x_0, x_3]$, $[x_0, x_4]$, and $[x_0, x_5]$, respectively; that is,

$|f^{(n+1)}(x)| \leq M_{n+1}$ for $x_0 < x < x_n$,

for $n = 1, 2, 3, 4, 5$. The error terms corresponding to these three cases have the following useful bounds on their magnitude

(i) $|R_1(x)| \leq \frac{M_2}{8} h^2$ is valid for $x \in [x_0, x_1]$,

(ii) $|R_2(x)| \leq \frac{M_3}{9\sqrt{3}} h^3$ is valid for $x \in [x_0, x_2]$,

(iii) $|R_3(x)| \leq \frac{M_4}{24} h^4$ is valid for $x \in [x_0, x_3]$,

(iv) $|R_4(x)| \leq \frac{\sqrt{4750 + 290\sqrt{145}}}{3000} M_5 h^5$ is valid for $x \in [x_0, x_4]$

(V) $|R_5(x)| \leq \frac{10 + 7\sqrt{7}}{1215} M_6 h^5$ is valid for $x \in [x_0, x_5]$.

Newton's Forward Interpolation Error:

It can be readily shown that the error at any is:

$$e(x) = f(x) - g(x) = \frac{(x - x_0)(x - x_1) \cdots (x - x_N)}{(N+1)!} f^{(N+1)}(\xi) \qquad x_0 < \xi < x_N$$

This error function is identical to that for Lagrange Interpolation (since the polynomial approximation is the same).

However we note that $f^{N+1}(x)$ can be approximated as

$$f^{(N-1)}(x_0) \cong \frac{\Delta^{N-1} f_0}{h^{N+1}}$$

In fact if $f^{N+1}(x)$ does not vary dramatically over the interval

$$f^{(N+1)}(\xi) \cong \frac{\Delta^{N+1} f_0}{h^{N-1}}$$

Thus the error can be estimated as

$$e(x) \cong \frac{(x-x_0)(x-x_1)\cdots(x-x_N)}{(N+1)!}\,\frac{\Delta^{N+1} f_0}{h^{N+1}}$$

Approximation for $e(x)$ is equal to the term that would follow the last term in the Nth degree polynomial series for $g(x)$.

If we have $N + 2$ data points available and develop an N^{th} degree polynomial approximation with $N + 1$ data points, we can then easily estimate $e(x)$. This was not as simple for Lagrange polynomials since you then needed to compute the finite difference approximation to the derivative in the error function.

If the exact function $f(x)$ is a polynomial of degree $M \le N$, then $g(x)$ will be an (almost) exact representation of $f(x)$ (with small round off errors).

i.e., Error in Newton's Forward Interpolation formula:

$$R_n = \frac{s(s-1)(s-2)\cdots(s-n)}{(n+1)!}\Delta^{n+1} f(x_0), \text{ where } s = \frac{x-x_0}{h}.$$

Newton's Backward Interpolation Error:

The difference between the interpolated value and the actual value is known as error in the polynomial interpolation. This determines the accuracy of the interpolation formula.

Error in Newton's Backward Interpolation formula:

$$R_n = \frac{s(s+1)(s+2)\cdots(s+n)}{(n+1)!}\nabla^{n+1} f(x_0+nh)., \text{ where } s = \frac{x-x_0}{h}.$$

Newton Interpolation is much more efficient to implement than Lagrange Interpolation.

3.7 Fitting of Polynomials and Other Curve

Curve Fitting: Curve fitting is finding a curve which matches a series of data points and possibly other constraints. Field data is often accompanied by noise. Even though all control parameters (independent variables) remain constant, the resultant outcomes (dependent variables) vary. A process of quantitatively estimating the trend of the outcomes, also known as *regression or curve fitting*, therefore becomes necessary.

Fitting Lines and Polynomial Curves to Data Points:

Let's start with a first degree polynomial equation:

$$y = ax + b$$

This is a line with slope *a*. We know that a line will connect any two points. So, a first degree polynomial equation is an exact fit through any two points.

If we increase the order of the equation to a second degree polynomial, we get:

$$y = ax^2 + bx + c$$

This will exactly fit three points.

If we increase the order of the equation to a third degree polynomial, we get:

$$y = ax^3 + bx^2 + cx + d$$

This will exactly fit four points. A more general statement would be to say it will exactly fit four **constraints**.

Fitting other curves to data points:

Other types of curves, such as conic sections (circular, elliptical, parabolic, and hyperbolic arcs) or trigonometric functions (such as sine and cosine), may also be used, in certain cases.

Curve fitting is nothing but approximating the given function **f(x)** using simpler functions say polynomials, trigonometric functions, exponential functions and rational functions. However, the main difference between interpolation and Curve fitting is, in the former, the approximated curve has to pass through the given data points. Here again polynomial functions are the one which are been used widely in the applications than the other functions.

3.8 Least Square Approximation of Functions

The curve fitting process fits equations of approximating curves to the raw field data. Nevertheless, for a given set of data, the fitting curves of a given type are generally *NOT unique*. Thus, a curve with a minimal deviation from all data points is desired. This *best-fitting curve* can be obtained by *the method of least squares*.

The method of least squares assumes that the best-fit curve of a given type is the curve that has the minimal sum of the deviations squared (*least square error*) from a given set of data.

Suppose that the data points are,

(x_1, y_1), (x_2, y_2), ..., (x_n, y_n) where x is the independent variable and y is the dependent variable. The fitting curve $f(x)$has the deviation (error) d from each data point,

i.e., $d_1 = y_1 - f(x_1)$, $d_2 = y_2 - f(x_2)$, ..., $d_n = y_n - f(x_n)$.

According to the method of least squares, the best fitting curve has the property that:

$$\Pi = d_1^2 + d_2^2 + \ldots + d_n^2 = \sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} [y_i - f(x_i)]^2 = \text{a minimum}$$

3.9 LINEAR AND POLYNOMIAL REGRESSION

Regression:

In regression analysis, *least squares*, also known as *ordinary least squares* analysis is a method for linear regression that determines the values of unknown quantities in a statistical model by minimizing the sum of the residuals (difference between the predicted and observed values) squared. Today, this method is available in most statistical packages. Furthermore, many other types of optimization problems can be expressed in a least squares form, by either minimizing energy or maximizing entropy. *The Least squares line* is often times called the line of *Regression*. Polynomials are one of the most commonly used types of curves in regression.

Linear Regression:

Linear regression analyzes the relationship between two variables, X and Y. For each subject (or experimental unit), you know both X and Y and you want to find the best straight line through the data. In some situations, the slope and/or intercept have a scientific meaning. In other cases, you use the linear regression line as a standard curve to find new values of X from Y, or Y from X.

The term "regression", like many statistical terms, is used in statistics quite differently than it is used in other contexts. The term "regression" is now used for many sorts of curve fitting.

In general, the goal of linear regression is to find the line that best predicts Y from X. Linear regression does this by finding the line that minimizes the sum of the squares of the vertical distances of the points from the line.

Polynomial Regression:

Polynomial regression fits data to this equation:

$$Y = A + B \cdot X + C \cdot X^2 + D \cdot X^3 + E \cdot X^4 \ldots$$

You can include any number of terms. If you stop at the second (B) term, it is called a first-order polynomial equation, which is identical to the equation for a straight line. If you stop after the third (C) term, it is called a second-order, or quadratic, equation. If you stop after the fourth term, it is called a third-order, or cubic, equation. If you choose a second, or higher, order equation, the graph of Y vs. X will be curved (depending on your choice of A, B, C...). vs. Y would be linear. From a mathematical point of view, the polynomial equation is linear.

Polynomial regression can be useful to create a standard curve for interpolation, or to create a smooth curve for graphing.

Multiple Regressions:

Multiple Regressions fits data to a model that defines Y as a function of two or more independent (X) variables. For example, a model might define a biological response as a function of both time and concentration. The term *multiple regression* is usually used to mean fitting data to a linear equation with two or more X variables (X1, X2, ...).

$$Y = A + B \cdot X_1 + C \cdot X_2 + D \cdot X_3 + E \cdot X_4 \ldots$$

Nonlinear multiple regression models define Y as a function of several X variables using a more complicated equation.

The Least-Squares Line (Linear Fitting):

The least-squares line uses a straight line $y = a + bx$ to approximate the given set of data, $(x_1, y_1), (x_2, y_2), \cdots, (x_n, y_n)$, where $n \geq 2$. The best fitting curve $f(x)$ has the least square error, i.e.,

$$\Pi = \sum_{i=1}^{n} [y_i - f(x_i)]^2 = \sum_{i=1}^{n} [y_i - (a + bx_i)]^2 = \min.$$

The unknown coefficients a and b can be obtained:

$$a = \frac{\sum_{i=1}^{n} y \sum_{i=1}^{n} x^2 - \sum_{i=1}^{n} x \sum_{i=1}^{n} xy}{n\sum_{i=1}^{n} x^2 - \left(\sum_{i=1}^{n} x\right)^2}$$

$$b = \frac{n\sum_{i=1}^{n} xy - \sum_{i=1}^{n} x \sum_{i=1}^{n} y}{n\sum_{i=1}^{n} x^2 - \left(\sum_{i=1}^{n} x\right)^2}$$

Example 3.7

Find the least-squares line y = a+ bx for the data

x	-2	-1	0	1	2
y	1	2	3	3	4

Solution:

Here $n = 5$,

a and b can be obtained by,

$$a = \frac{\sum_{i=1}^{n} y \sum_{i=1}^{n} x^2 - \sum_{i=1}^{n} x \sum_{i=1}^{n} xy}{n\sum_{i=1}^{n} x^2 - \left(\sum_{i=1}^{n} x\right)^2}$$

$$b = \frac{n\sum_{i=1}^{n} xy - \sum_{i=1}^{n} x \sum_{i=1}^{n} y}{n\sum_{i=1}^{n} x^2 - \left(\sum_{i=1}^{n} x\right)^2}$$

X	***Y***	***X²***	***xy***
-2	1	4	-2
-1	2	1	-2
0	3	0	0
1	3	1	3
2	4	4	8
$\sum x = 0$	$\sum y = 13$	$\sum x^2 = 10$	$\sum xy = 7$

Hence $a = \frac{13 \times 10 - 0 \times 7}{5 \times 10 - 0^2}$

$$= \frac{130}{50}$$

$$= 2.6$$

$$b = \frac{5 \times 7 - 0 \times 13}{5 \times 7 - 0^2}$$

$$= \frac{35}{50}$$

$$= 0.7$$

$y = 2.6 + 0.7x$ or $y = 0.7x + 2.6$

Fitting a Second Degree Parabola Using Least Squares Line (Polynomial Fitting):

The least-squares parabola uses a second degree curve

$y = a + bx + cx^2$ to approximate the given set of data,

$(x_1, y_1), (x_2, y_2) \cdots (x_n, y_n)$, where $n \geq 3$.

The best fitting curve $f(x)$ as the least square error, i.e.,

$$\Pi = \sum_{i=1}^{n} [y_i - f(x_i)]^2 = \sum_{i=1}^{n} \left[y_i - (a + bx_i + cx_i^{\,2})\right]^2 = \min$$

The unknown coefficients a, b, and c can hence be obtained by solving the below linear equations.

$$\sum_{i=1}^{n} y_i = na + b\sum_{i=1}^{n} x_i + c\sum_{i=1}^{n} x_i^2$$

$$\sum_{i=1}^{n} x_i y_i = a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 + c\sum_{i=1}^{n} x_i^3$$

$$\sum_{i=1}^{n} x_i^2 y_i = a\sum_{i=1}^{n} x_i^2 + b\sum_{i=1}^{n} x_i^3 + c\sum_{i=1}^{n} x_i^4$$

Example 3.8

Find the least-squares parabolic $y = a + bx + cx^2$ for the data

X	-3	-1	1	3
y	15	5	1	5

Solution:

Here $n = 4$ and

a, b and c obtained by solving the below equation,

$$\sum_{i=1}^{n} y_i = na + b\sum_{i=1}^{n} x_i + c\sum_{i=1}^{n} x_i^2$$

$$\sum_{i=1}^{n} x_i y_i = a\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 + c\sum_{i=1}^{n} x_i^3$$

$$\sum_{i=1}^{n} x_i^2 y_i = a\sum_{i=1}^{n} x_i^2 + b\sum_{i=1}^{n} x_i^3 + c\sum_{i=1}^{n} x_i^4 .$$

x	y	x^2	x^3	x^4	xy	$x^2 y$
-3	15	9	-27	81	-45	135
-1	5	1	-1	1	-5	5
1	1	1	1	1	1	1
3	5	9	27	81	15	45
$\sum x = 0$	$\sum y = 26$	$\sum x^2 = 20$	$\sum x^3 = 0$	$\sum x^4 = 164$	$\sum xy = -34$	$\sum x^2 y = 186$

The resulting linear system for determining a, b, and c is

$$4a + 0b + 2c = 26$$

$$20b = -34$$

$$20a + 0b + 164c = 186$$

The solution to linear system $a = 2.125$, $b = -1.7$ and $c = 0.875$.

Hence,

$y = 2.125 - 1.7x + 0.875x^2$ or

$y = 0.875x^2 - 1.7x + 2.125$.

Fitting *m*th Degree Polynomials using Least-Squares Line:

When using an m^{th} degree polynomial $y = a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m$ to approximate the given set of data, $(x_1, y_1), (x_2, y_2) \cdots (x_n, y_n)$, where $n \ge m+1$, the best fitting curve $f(x)$ has the least square error, i.e.,

$$\Pi = \sum_{i=1}^{n} [y_i - f(x_i)]^2 = \sum_{i=1}^{n} \left[y_i - (a_0 + a_1 x_i + a_2 x_i^2 + \ldots + a_m x_i^m) \right]^2 = \min.$$

Please note that $a_0, a_1, a_2, \cdots,$ and a_m are unknown coefficients while all x_i and y_i are given. The unknown coefficients $a_0, a_1, a_2, \cdots,$ and a_m can hence be obtained by solving the below linear equations.

$$\sum_{i=1}^{n} y_i = na_0 + a_1 \sum_{i=1}^{n} x_i + a_2 \sum_{i=1}^{n} x_i^2 + \cdots + a_m \sum_{i=1}^{n} x^m{}_i$$

$$\sum_{i=1}^{n} x_i y_i = a_0 \sum_{i=1}^{n} x_i + a_1 \sum_{i=1}^{n} x_i^2 + a_2 \sum_{i=1}^{n} x_i^3 + \cdots + a_m \sum_{i=1}^{n} x_i^{m+1}$$

$$\sum_{i=1}^{n} x_i^2 y_i = a_0 \sum_{i=1}^{n} x_i^2 + a_1 \sum_{i=1}^{n} x_i^3 + a_2 \sum_{i=1}^{n} x_i^4 + \cdots + a_m \sum_{i=1}^{n} x_i^{m+2}$$

$\vdots$

$\vdots$

$$\sum_{i=1}^{n} x_i^m y_i = a_0 \sum_{i=1}^{n} x_i^m + a_1 \sum_{i=1}^{n} x_i^{m+1} + a_2 \sum_{i=1}^{n} x_i^{m+2} + \cdots + a_m \sum_{i=1}^{n} x_i^{2m}$$

Data Linearization Method for Exponential Curve Fitting (Nonlinear Curve Fitting):

Fit the curve $y = ce^{bx}$ to the data points

$(x_1, y_1), (x_2, y_2) \cdots (x_n, y_n)$.

Taking the logarithm of both sides we obtain

$$\ln(y) = \ln(c) + \ln(e^{bx}) = \ln(c) + bx$$

$$\ln(y) = \ln(c) + bx$$

Introduce the change of variable, $X = x$, $Y = \ln(y)$, $B = b$ and $A = \ln(c)$. Then the previous equation becomes, $Y = A + BX$ which is a linear equation in the variable X and Y.

Use the change of variables $X = x$ and $Y = \ln(y)$ on all the data points and obtain

$$X_k = x_k \text{ and } Y_k = \ln(y_k) \text{ for } k = 1, 2, \ldots, n.$$

This process is called *Data Linearization.*

Fit the points $(x_1, y_1), (x_2, y_2) \cdots (x_n, y_n)$ with a Least-Squares line of the form $Y = A + BX$.

Comparing the equations $Y = A + BX$ and $Y = \ln(c) + BX$ we see that $A = \ln(c)$ and $B = b$. Thus $b = B$ and $c = e^A$ are used to construct the coefficients which are then used to "fit the curve" $y = ce^{bx}$ to the given points $(x_1, y_1), (x_2, y_2) \cdots (x_n, y_n)$ in the xy-plane.

Example 3.9

Use the data linearization method and find the exponential fit $y = ce^{bx}$, for the data points (1,0.6), (2,1.9), (3,4.3), (4,7.6) and (5, 1.6094).

Solution:

By data linearization, the original points (x_k, y_k) in the xy-plane are transformed into $(X_k, Y_k) = (x_k, \ln(y_k))$ in $XY-$ plane. Hence,

$$\{(X_k, Y_k)\} = \{(x_k, \ln(y_k))\}$$

$$= \{(1, \ln(0.6)), (2, \ln(1.9)), (3, \ln(4.3)), (4, \ln(7.6)), (5, \ln(12.6))\}$$

$$= \{(1, \ln(0.6)), (2, \ln(1.9)), (3, \ln(4.3)), (4, \ln(7.6)), (5, \ln(12.6))\}$$
$$= \{(1, -.5108), (2, 0.6419), (3, 1.4586), (4, 2.0281), (5, 2.5337)\}$$

By Least-Square Lines $y = ce^{bx}$ becomes,

$Y = A + BX$ where $Y = \ln(c) + BX$, $A = \ln(c)$ and $B = b$.

We can obtain the value of A and B by solving below equations,

$$A = \frac{\sum_{i=1}^{n} Y \sum_{i=1}^{n} X^2 - \sum_{i=1}^{n} X \sum_{i=1}^{n} XY}{n\sum_{i=1}^{n} X^2 - \left(\sum_{i=1}^{n} X\right)^2}$$

$$B = \frac{n\sum_{i=1}^{n} XY - \sum_{i=1}^{n} X \sum_{i=1}^{n} Y}{n\sum_{i=1}^{n} X^2 - \left(\sum_{i=1}^{n} X\right)^2}$$

where $n = 5$,

$X_k = x_k$	y_k	$Y_k = \ln(y_k)$	X_k^2	$X_k Y_k$
1	0.6	-0.5108	1	-0.5108
2	1.9	0.6419	4	1.2838
3	4.3	1.4586	9	4.3758
4	7.6	2.0281	16	8.1124
5	12.6	2.5337	25	12.6685
$\sum X_k = 15$	$\sum y_k = 27$	$\sum Y_k = 6.1515$	$\sum X^2 = 55$	$\sum X_k Y_k =$ 25.9297

Hence $A = \dfrac{6.1515 \times 55 - 15 \times 25.9297}{5 \times 55 - 15^2} = -1.0123$

$$B = \frac{5 \times 25.9297 - 15 \times 6.1515}{5 \times 55 - 15^2} = 0.7474$$

We know that $b = B$ and $c = e^A$ are used to construct the coefficients which are then used to "fit the curve" $y = ce^{bx}$ to the given points $(x_1, y_1), (x_2, y_2) \cdots (x_n, y_n)$ in the xy-plane.

$$\therefore c = e^A = e^{-1.0123} = 0.3634$$

The required equation is $y = 0.3634e^{0.7474x}$.

KEY WORDS

Keywords: Quadrature, Cubature, Definite Integral, Derivative, Polynomials, Slope, Tangent, Mid-Point, Taylor- Series, Extrapolation, Argument, Adjacent, Remainder, Accuracy, Curve, Linear, Parabola, Regression.

LEARNING ACTIVITIES

a) Fill in the blanks:

1) _________is a method of constructing new data points from a discrete set of known data points

2) The difference between the interpolated value and the actual value is known as_______ in the polynomial interpolation

b) State whether true or false:

1) Lagrange's formula is more convenient to use in computer programming

2) This *best-fitting curve* can be obtained by *the method of least squares.*

Answer to learning Activities

a) Fill in the blanks:

1) *interpolation*
2) error

b) State whether true or False:

1) true
2) true

Model Questions

1. Define Interpolation.
2. Write note on Extrapolation.
3. Using Lagrange's formula find the value of y when $x = 3$. The values of x and y are:

x	0	1	2	5
y	2	3	12	147

4. Discuss Inverse Interpolation.
5. Using Lagrange's Inverse Interpolation formula find the value of x when y = 19. The values of x and y are:

y	1	3	4
x	4	12	19

6. What do you mean by Divided and Difference Method?

7. Construct the Divided Difference for the following data:

x	1	2	4	7	10
$f(x)$	5	10	26	65	122

8. Given

x	2	3	4	5
$f(x)$	2.626	3.454	4.784	6.986

find $f(3.5)$ using Newton's Interpolation formula.

9. Explain Interpolation at Equally spaced points.

10. Given

x	2.5	3.0	3.5	4.0	4.5	5.0
$f(x)$	24.145	22.043	20.225	18.644	17.262	16.047

find $f(3.75)$ using Newton's Forward Difference formula.

11. Given

x	20	30	40	50	60	70
$f(x)$	0.342	0.502	0.642	0.766	0.866	0.939

find $f(45)$ using Newton's Backward Difference formula.

12. Discuss Errors of the Interpolating Polynomials.

13. Define Curve Fitting.

14. Discuss different types of Regression.

15. Write note on Least-Square Method.

16. Find the least-squares line $y = a + bx$ for the data

x	y
-1	10
0	9
1	7
2	5
3	4
4	3
5	0
6	-1

17. Find the least-squares parabolic $y = a + bx + cx^2$ for the data:

x	-3	0	2	4
y	3	1	1	3

18. Use the data linearization method and find the exponential fit $y = ce^{bx}$, for the data points (0, 1.5), (1, 2.5), (2, 3.5), (3, 5.0), and (4, 7.5).

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Block 4: Introduction

In this block, we will learn about the basics of numerical differentiation and integration. We earn knowledge of trapezoidal rule, simpson's rule and finally euler's rule. This block is divided into one unit are as follows.

Unit 4: it deals with numerical differentiation and integration.

UNIT-4

NUMERICAL DIFFERENTIATION AND INTEGRATION

Structure

Overview

Learning Objectives

4.1 Numerical Integration

4.2 The Trapezoidal Rule

4.3 Simpson's one-third Rule

4.4 Simpson's Three Eighth Rule

4.5 Gaussian Quadratic Formula

4.6 Numerical Solution of Differential Equations

4.7 Euler's Method

4.8 Runge-Kutta Methods

Keywords

Answer to Learning Activities

References

OVERVIEW

In numerical analysis, *Numerical Integration* constitutes a broad family of algorithms for calculating the numerical value of a definite integral, and by extension, the term is also sometimes used to describe the numerical solution of differential equations. This unit focuses on calculation of definite integrals. The term *Quadrature* is more or less a synonym for *numerical integration*, especially as applied to one-dimensional integrals. Two- and higher-dimensional integration is sometimes described as *Cubature*, although the meaning of *quadrature* is understood for higher dimensional integration as well.

Numerical ordinary differential equation is the part of numerical analysis which studies the numerical solution of ordinary differential equations (ODEs). This field is also known under the name *numerical integration,* but some people reserve this term for the computation of integrals.

Many differential equations cannot be solved analytically, in which case we have to satisfy ourselves with an approximation to the solution. The algorithms studied here can be used to compute such an approximation. An alternative method is to use techniques from calculus to obtain a series expansion of the solution.

Ordinary differential equations occur in many scientific disciplines, for instance in mechanics, chemistry, biology, and economics. In addition, some methods in numerical partial differential equations convert the partial differential equation into an ordinary differential equation, which must then be solved.

LEARNING OBJECTIVES

After studying this unit, you should be able to discuss about

- Numerical Integration
- To find approximate solution of an Integral Domain using Trapezoidal, Simpson's one-third, and Simpson's 3/8 rule.
- The Gaussian Quadrature and their basic rules
- Various forms of Gaussian Quadrature
- To explain Differential Equation

- Discuss Euler's Method, Improved Euler's Method and Modified Euler's Method

4.1 NUMERICAL INTEGRATION

There are several reasons for carrying out numerical integration. The integrand *f* may be known only at certain points, such as obtained by sampling. Some embedded systems and other computer applications may need numerical integration for this reason.

The basic problem considered by numerical integration is to compute an approximate solution to a definite integral:

$$\int_a^b f(x)dx.$$

The Newton-Cotes Integration, most commonly used numerical integration methods are,

- The Trapezoidal Rule
- Simpson's one-third Rule
- Simpson's Three Eighth Rule
- Gaussian Quadratic Formula

These commonly used numerical integration method, approximate the integration of a complicated function by replacing the function with many *polynomials* across the integration interval. The integration of the original function can then be obtained by summing up all polynomials whose "areas" are calculated by the weighting coefficients and the values of the function at the nodal points.

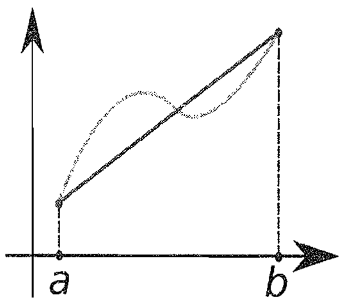
4.2 THE TRAPEZOIDAL RULE

The trapezoidal rule is a method for finding an approximate value for a definite integral. Suppose we have the definite integral

$$\int_a^b f(x)dx.$$

First the area under the curve $y = f(x)$ is divided into ***n*** strips, each of equal width

$$h = \frac{b-a}{n}$$



The function f(x) is approximated by a linear function.

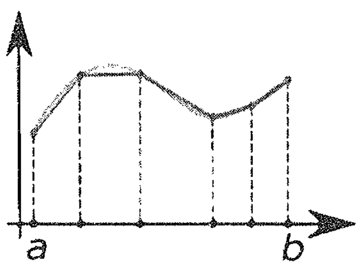


Illustration of Composite Trapezium Rule.

The shape of each strip is approximated to be like that of a trapezium. Hence the area of the first strip is approximately

$$\int_a^b f(x)dx = (b-a)\frac{f(a)+f(b)}{2} \quad = \frac{h}{2}(y_0 + y_1)$$

where $y_0 = f(a) \& y_1 = f(b)$.

The Trapezium Rule estimates the area under a curve between limits by turning the curve into a set of trapeziums (or strips) and each strip is made out of two ordinates, so there is always one more ordinates than there are strips. The formula is:

$$\int_a^b y\,dx \approx \frac{h}{2}\{(y_0+y_n)+2(y_1+y_2+\cdots+y_{n-1})\}$$

Where $h = (b-a)/n$

Example

Use Trapezoidal Rule to evaluate the approximate values of the definite integrals:

$$\int_0^1 \sin x \, dx.$$

Given that

X	0	0.2	0.4	0.6	0.8	1.0
$f(x)$	0	0.1987	0.3894	0.5646	0.7174	0.8415

Solution:

The Trapezoidal formula is:

$$\int_a^b y\,dx \approx \frac{h}{2}\{(y_0+y_n)+2(y_1+y_2+\cdots+y_{n-1})\}$$

We shall divide the interval into 5 strips each of width

$$h = \frac{b-a}{n} = \frac{1-0}{5} = 0.2$$

By Trapezoidal Rule,

$$\int_0^1 \sin x dx = \frac{0.2}{2}\{(\sin 0 + \sin 1) + 2(\sin 0.2 + \sin 0.4 + \sin 0.6 + \sin 0.8)\}$$

$$= 0.45817.$$

4.3 SIMPSON'S ONE-THIRD RULE

Simpson's rules generalize the trapezoidal rule to use more than two points per interval, so we can use quadratic or cubic models instead of linear. For a single interval, we will derive Simpson's 1/3 rule.

We will need to find the quadratic equation that goes through three points (x_1, $f(x_1)$), (x_2, $f(x_2)$), (x_3, $f(x_3)$). We will then integrate the quadratic to obtain the estimate of the integral. This also integrates cubic exactly.

Divide the interval [a, b] into n equal segments, each of width (b-a)/n.

•Apply the Simpson's 1/3 rule to each pair of segments

•Add up all the results

•This is more accurate than the trapezoidal rule.

Simpson's Rule is formed by approximating a general curve by a parabola. We won't show you how to determine the coefficients for the parabola, but it is fairly straightforward. As before, the width of each of the two intervals is

$$h = \frac{b-a}{2}$$

With a little bit of work, you would find the approximation,

$$\int_a^b f(x) = s_1 = \frac{h}{3}[y_0 + 4y_1 + y_2]$$

This is Simpson's Rule with one step. More generally, we can break the interval into several pieces and apply Simpson's Rule on each interval. For instance, to use n steps, break the interval $[a,b]$ into $2n$ pieces, each of width $h = \frac{b-a}{2n}$. Call the x coordinates $x_0, x_1, \cdots, x_{2n-1}, x_{2n}$ and let $y_i = f(x_i)$. Then we have,

$$\int_a^b f(x)\, dx = s_n = \frac{h}{3}[y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \cdots + 4y_{2n-1} + y_{2n}]$$

$$= \frac{h}{3}[(y_0 + y_{2n}) + 4(y_1 + y_3 + \cdots y_{2n-1}) + 2(y_2 + y_4 + \cdots y_{2n-2})]$$

Example

Apply Simpson's one-third ($\frac{1}{3}$) rule to evaluate $\int_2^{10} \frac{dx}{1+x}$ by dividing the range into 4 equal parts.

Solution:

Here $h = \frac{10-2}{4} = \frac{8}{4} = 2$,

the computed values of $y = \frac{1}{1+x}$ are tabulated as

X	2	4	6	8	10
Y	.333	.20	.143	.111	.091

By Simpson's One-third Rule,

$$\int_a^b \frac{dx}{1+x} = \frac{2}{3}[(.333+.091)+4(0.2+0.111)+2(.143)]$$

$$\approx 1.30$$

4.4 SIMPSON'S 3/8 RULE

Let the values of a function f(x) be tabulated at points x_i equally spaced by

$h = x_{i+1} - x_i$, so $y_0 = f(x_0), y_1 = f(x_1), \cdots, y_3 = f(x_3)$.

Then Simpson's 3/8 rule approximating the integral of $f(x)$ is given by the Newton-Cotes-like formula,

$$\int_a^b f(x) = \frac{3h}{8}[(y_0 + y_1) + 3(y_2 + y_3)]$$

The result can be extended by taking ***n*** (a multiple of 3), intervals each of length ***h*** is,

$$\int_a^b f(x) = \frac{3h}{8}[(y_1 + y_n) + 3(y_1 + y_2 + y_4 + y_5 + \cdots + y_{n-1}) + 2(y_1 + y_6 + \cdots y_{n-3})]$$

Example

Evaluate $\int_0^6 \frac{1}{1+x^2} dx$ into 6 equal parts by Simpson's 3/8 Rule.

Solution:

Here h = 1, and n = 6.

Now the computed values of y are,

X	0	1	2	3	4	5	6
Y	1.00	0.5	0.2	0.1	0.05882	0.03846	0.02702

$$\int_0^6 \frac{1}{1+x^2}dx = \frac{3}{8}\times 1\times[(1.00+0.02707)+3(0.5+0.2+0.05882+0.3846)+2\times 0.1]$$

$$= 1.35708$$

4.5 GAUSSIAN QUADRATURE

In numerical analysis, a *quadrature rule* is an approximation of the definite integral of a function, usually stated as a weighted sum of function values at specified points within the domain of integration.

An *n*-point *Gaussian quadrature rule*, named after Carl Friedrich Gauss, is a quadrature rule constructed to yield an exact result for polynomials of degree $2n - 1$, by a suitable choice of the n points x_i and n weights w_i. The domain of integration for such a rule is conventionally taken as [−1, 1], so the rule is stated as

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

Rules for the basic problem

For the integration problem stated above, the associated polynomials are Legendre polynomials. Some low-order rules for solving the integration problem are listed below.

Number of points, n	Points, x_i	Weights, w_i
1	0	2
2	$\pm\sqrt{1/3}$	1
3	0	8/9
	$\pm\sqrt{3/5}$	5/9
4	±0.339981044	0.652145155
	±0.861136312	0.347854845
5	0	0.568889
	±0.538469	0.478629
	±0.906180	0.236927

Change of interval for Gaussian quadrature:

An integral over [a, b] must be changed into an integral over [−1, 1] before applying the Gaussian quadrature rule. This change of interval can be done in the following way:

$$\int_a^b f(t)\,dt = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}x + \frac{a+b}{2}\right)dx$$

After applying the Gaussian quadrature rule, the following approximation is obtained:

$$\frac{b-a}{2}\sum_{i=1}^{n} w_i f\left(\frac{b-a}{2}x_i + \frac{a+b}{2}\right)$$

Other forms of Gaussian Quadrature:

The integration problem can be expressed in a slightly more general way by introducing a positive weight function *w* into the integrand, and allowing an interval other than [−1, 1].

That is, the problem is to calculate

$$\int_a^b w(x) f(x)\, dx$$

for some choices of *a*, *b*, and ω. For *a* = −1, *b* = 1, and *w*(*x*) = 1, the problem is the same as that considered above. Other choices lead to other integration rules.

Gaussian quadrature also comes in other forms: Laguerre, Hermite, Chebychev, etc. for functions with infinite limits of integration, or which are not finite in the interval Gauss Quadrature or Gauss Legendreis highly accurate with a small number of points suitable for continuous functions on closed intervals.

Interval	*w(x)*	Orthogonal polynomials
[−1, 1]	1	Legendre polynomials
(−1, 1)	$\frac{1}{\sqrt{1-x^2}}$	Chebyshev polynomials (first kind)
[−1, 1]	$\sqrt{1-x^2}$	Chebyshev polynomials (second kind)
[0, ∞)	e^{-x}	Laguerre polynomials
(−∞, ∞)	e^{-x^2}	Hermite polynomials

4.6 NUMERICAL SOLUTION OF A DIFFERENTIAL EQUATIONS

The numerical methods for solving ordinary differential equations (ODE's) are methods of *integrating a system of first order differential equations*, since higher order ordinary differential equations can be reduced to a set of first order ODE's.

An ordinary differential equation is an equality involving a function and its derivatives. An ODE of order n is an equation of the form $F(x, y', y^2, \cdots y^n) = 0$, where y is a function of x, $y^1 = dy/dx$ is the first derivative with respect to x, and $y^n = d^n y/dx^n$ is the nth derivative with respect to x

Common numerical methods for solving *initial value problems* of ordinary differential equations are:

- Euler's Method
- Runge-Kutta Method

The Numerical Solution of Differential Equations covers a wide variety of mathematical topics and technical skills, with a variety of potential applications and career opportunities.

4.7 EULER'S METHOD

Euler's Method:

The simplest method of numerical integration is Euler's method.

In order to develop a technique for solving first order initial value problems numerically, we should first agree upon some notation. We will assume that the problem in question can be algebraically manipulated into the form:

$$y_1 = f(x, y)$$

Remember that one interpretation of the quantity y_1 appearing in this expression is as the *slope of the tangent line* to the function *y*. But, the function *y* is exactly what we are seeking as a solution to the problem.

$\therefore$ Slope of the solution = $f(x, y)$.

We start at the point (x_0, y_0).

Let *h* denote the *x*-increment.

Then $x_1 = x_0 + h.y_1$ is the *y*-coordinate of the point on the line passing through the point (x_0, y_0) with slope $y_1(x_0) = f(x_0, y_0)$. **Thus,** $y_1 = y_0 + h.f(x_0, y_0)$.

The next approximation is found by replacing x_0 and y_0 by x_1 and y_1; so $x_2 = x_1 + h$. **Thus,** $y_2 = y_1 + h.f(x_1, y_1)$.

In general, we obtain the following formula for $\mathrm{n} = 1, 2, 3, \ldots,$

$$x_n = x_{n-1} + h = x_0 + n.h,$$
$$y_n = y_{n-1} + h.f(x_{n-1}, y_{n-1}).$$

Example

Use Euler's Method to approximate y when $x = 0.5$, given that $y' = -2x - y,$ with y = -1 fox x =0.

Solution:

Here $y' = \dfrac{dy}{dx} = -2x - y$

With $y_0 = -1$ when $x_0 = 0$ and take $h = 0.1$

$y_1 = y_0 + h\, f(x_0, y_0) = -1 + 0.1*(-2*0 - (-1)) = -0.8999$

$y_2 = y_1 + h\, f(x_1, y_1) = -0.8999 + 0.1*(-2*0 - (-0.8999)) = -0.8299$

$y_3 = y_2 + h\, f(x_2, y_2) = -0.8299 + 0.1*(-2*0 - (-0.8299)) = -0.7869$

$y_4 = y_3 + h\, f(x_3, y_3) = -0.7869 + 0.1*(-2*0 - (-0.7869)) = -0.7683$

$y_5 = y_4 + h\, f(x_4, y_4) = -0.7683 + 0.1*(-2*0 - (-0.7683)) = -0.7715$

Hence $y = -0.7715$ for $x = 0.5$.

Midpoint method Or Improved Euler's Method:

The Midpoint Method or improved Euler's Method is a one-step method for solving the differential equation

$y_1(x) = f(x, y(x)),\ \ y(x_0) = y_0$ and is given by the formula,

$$y_n = y_{n-1} + hf[x_{n-1} + \frac{h}{2}, y_{n-1} + \frac{h}{2} f(x_{n-1}, y_{n-1})] \text{ for } n = 0,1,2,\ldots$$

Here, h is the step size a small positive number, $x_n = x_0 + n.h$, and y_n is the computed approximate value of $y(x_n)$.

The name of the method comes from the fact that in the formula above the function f is evaluated at

$$x = x_n + h/2,$$

Which is the midpoint between x_n at which th e value of $y(x)$ is known and x_{n+1} at which the value of $y(x)$ needs to be found.

Example

Use Euler's Improved Method to solve $\frac{dy}{dx} = -y$ for $0 \le x \le 0.6$, and h=0.2 with the boundary condition y = 1 when x =0.

Solution:

Here $y' = \frac{dy}{dx} = -y = f(x, y)$

With $y_0 = 1$ when $x_0 = 0$ and take $h = 0.2$. $\therefore \frac{h}{2} = 0.1$.

Taking $y_1, y_2, y_3,$ as the approximations of y corresponding to

$x_1 = 0.2,\ x_2 = 0.4,\ x_3 = 0.6$ respectively,

we have,

$$y_1 = y_0 + hf[x_0 + \frac{h}{2}, y_0 + \frac{h}{2} f(x_0, y_0)]$$

$$= 1 + 0.2 f[0+0.1,1+0.1*(-1)]$$

$$= 0.82$$

$$y_2 = y_1 + hf[x_1 + \frac{h}{2}, y_1 + \frac{h}{2} f(x_1, y_1)]$$

$$= 0.82 + 0.2 f[0.3,.0738]$$

$$= 0.6724$$

$$y_3 = y_2 + hf[x_2 + \frac{h}{2}, y_2 + \frac{h}{2} f(x_2, y_2)]$$

$= 0.6724 + .2f[0.5, 0.60516]$

$= 0.551368.$

Hence $y = 0.551368$ at $x = 0.6$.

Modified Euler's Method:

The accuracy of Euler's method is improved by using an average of two slopes in the tangent line approximation.

Calculate $y_1^i = y_0 + h.f(x_0, y_0)$ and Calculate the slope $f(x_1, y_1^i)$ where $x_1 = x_0 + 1.h$, use the average of the two slopes.

$$y_1 = y_0 + (x_1 - x_0)\frac{f(x_0, y_0 + f(x_1, y_1^i)}{2}$$

$$= y_0 + h\frac{f(x_0, y_0) + f(x_1, y_1^i)}{2}$$

Continue this process.

Improved Euler's Method with step size h: The solution of the initial–value problem

$$\frac{dy}{dx} = f(x, y), \quad y(x_0) = y_0$$

is approximated at the sequence of points (x_n, y_n) ($n = 1,2,3\ldots$), where y_n is the approximate value of $y(x_n)$ by computing at each step the two calculations:

$$y_n^{i-1} = h.f(x_{n-1}, y_{n-1}) + y_{n-1}, \ (n = 1,2,3.....)$$

$$y_n^i = y_{n-1} + \frac{h}{2}[f(x_{n-1}, y_{n-1}) + f(x_n, y_n^{i-1})]$$

Where $x_n = x_0 + nh$ and h is selected step size.

Example

Use the Modified Euler's Method, Solve numerically the

$\frac{dy}{dx} = x + y$ with initial condition y=1, x =0 for range $0 \le x \le 0.4$ in

steps of 0.2.

Solution:

Given $\frac{dy}{dx} = x + y = (f\ x, y)$, $x_0 = 0,\ \ y_0 = 1,\ h = 0.2$

By Euler's Method,

$$y_n = y_{n-1} + h.f(x_{n-1}, y_{n-1})$$

$$y_1 = y_0 + h.f(x_0, y_0)$$

$$= 1 + 0.2\ f(0,1)$$

$$= 1.2$$

By Euler's Modified Method,

$$y_n^i = y_{n-1} + \frac{h}{2}[f(x_{n-1}, y_{n-1}) + f(x_n, y_n^{i-1})]$$

Put n = 1, i =1 in Euler Modified Method we have,

$x_1 = x_0 + h = 0 + 0.2 = 0.2$, and $y_1^0 = 1.2$,

$$y_1^1 = y_0 + \frac{h}{2}[f(x_0, y_0) + f(x_1, y_1^0)]$$

$$= 1.2 + \frac{0.2}{2}[f(0,1) + f(0.2, 1.2)]$$

$= 1.44$

$$y_1^2 = y_0 + \frac{h}{2}[f(x_0, y_0) + f(x_1, y_1^1)]$$

$$= 1.2 + \frac{0.2}{2}[f(0,1) + f(0.2, 1.44)]$$

$= 1.464$

$$y_1^3 = y_0 + \frac{h}{2}[f(x_0, y_0) + f(x_1, y_1^2)]$$

$$= 1.2 + \frac{0.2}{2}[f(0,1) + f(0.2, 1.464)]$$

$= 1.46642$

$$y_1^4 = y_0 + \frac{h}{2}[f(x_0, y_0) + f(x_1, y_1^3)]$$

$$= 1.2 + \frac{0.2}{2}[f(0,1) + f(0.2, 1.46642)]$$

$= 1.46664$

$$y_1^5 = y_0 + \frac{h}{2}[f(x_0, y_0) + f(x_1, y_1^4)]$$

$$= 1.2 + \frac{0.2}{2}[f(0,1) + f(0.2, 1.46664)]$$

$= 1.46666$

Hence $y_1 = 1.4666$ at $x = 0.2$.

To find y_2 by Euler's Method,

$$y_n = y_{n-1} + h.f(x_{n-1}, y_{n-1})$$

$$y_2 = y_1 + h.f(x_1, y_1)$$

$$= 1.4666 + 0.2\ f(0.2, 1.4666)$$

$$= 1.7999$$

By Euler's Modified Method,

$$y_n^i = y_{n-1} + \frac{h}{2}[f(x_{n-1}, y_{n-1}) + f(x_n, y_n^{i-1})]$$

Put n = 2, i =1 in Euler Modified Method we have,

$x_2 = x_1 + h = 0.2 + 0.2 = 0.4$, and $y_2^0 = 1.7999$,

$$y_2^1 = y_1 + \frac{h}{2}[f(x_1, y_1) + f(x_2, y_2^0)]$$

$$= 1.4666 + \frac{0.2}{2}[f(0.2, 1.4666) + f(0.4, 1.7999)]$$

$$= 1.8533$$

$$y_2^2 = y_1 + \frac{h}{2}[f(x_1, y_1) + f(x_2, y_2^1)]$$

$$= 1.4666 + \frac{0.2}{2}[f(0.2, 1.4666) + f(0.4, 1.8533)]$$

$$= 1.8586$$

$$y_2^3 = y_1 + \frac{h}{2}[f(x_1, y_1) + f(x_2, y_2^2)]$$

$= 1.4666 + \frac{0.2}{2}[f(0.2, 1.4666) + f(0.4, 1.8586)]$

$= 1.8591$

$$y_2^4 = y_1 + \frac{h}{2}[f(x_1, y_1) + f(x_2, y_2^3)]$$

$= 1.4666 + \frac{0.2}{2}[f(0.2, 1.4666) + f(0.4, 1.8586)]$

$= 1.8591$

Hence $y_2 = 1.8591$ at $x = 0.4$.

4.8 RUNGE-KUTTA METHOD

Runge-Kutta Method:

Runge-Kutta Method is the generalization of the concept used in Modified Euler's method.

Runge-Kutta Method of First Order:

The Euler's method can also be called Runge-Kutta method of first order. The Runge-Kutta Method is also called as RK Method. These methods agree with Taylor's series solution up to the terms of h^r where r is the order of RK Method.

By Euler's Method,

$$y_1 = y_0 + hf(x_0, y_0)$$

Also, $y_1 = y(x_0 + h) = y_0 + \frac{h}{\underline{|1}} y_0' + \frac{h}{\underline{|2}} y_0'' + \cdots$.

$\therefore$ The Euler's method agrees with the Taylor's series solution up to the term in h. Hence the Euler's Method is the Runge-Kutta method of first order.

Runge-Kutta Method of Order Two:

The Improved Euler's method can also be called Runge-Kutta method of order two.

The solution of the initial-value problem,

$\frac{dy}{dx} = f(x,y), \quad y(x_0) = y_0$ is approximated at the sequence of points $(x_n, y_n) \quad (n = 1,2,3,4,...)$, where y_n is the approximate value of $y(x_n)$ by computing at each step,

$$y_{n+1} = y_n + \frac{1}{2}(k_1 + k_2), \quad (n = 1,2,3,4,...),$$

with $k_1 = h.f(x_n, y_n)$,

$k_2 = h.f(x_n + h, y_n + k_1)$ and

$x_n = x_0 + n.h$

with h is the selected step size.

$\therefore$ The second order Runge-Kutta Method is $y = y + \frac{1}{2}(k_1 + k_2)$ where $k_1 = h.f(x_0, y_0)$ and $k_2 = h.f(x_0 + h, y_0 + k_1)$.

The Runge-Kutta Method of Order Three:

The third order Runge-Kutta formula is given by

$$y_1 = y_0 + \frac{1}{6}\left(k_1 + 4k_2 + k_3\right)$$

Where $k_1 = h.f(x_0, y_0)$,

$$k_2 = h.f(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}),$$

$$k_3 = h.f(x_0 + h, y_0 + k'),$$

Where $k' = h.f(x_0 + h, y_0 + k_1)$.

The Runge-Kutta Method of Order Four:

The fourth order of Runge-Kutta is

$$y = y + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

Where $k_1 = h.f(x_0, y_0)$,

$$k_2 = h.f(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2}),$$

$$k_3 = h.f(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2}),$$

$$k_4 = h.f(x_0 + h, y_0 + k_3).$$

Example

Apply Runge-Kutta Method to find the approximate value of y for x = 0.2 in step of 0.1 if $dy/dx = x + y^2$, given that y = 1, where x =0.

Solution:

Given $\frac{dy}{dx} = x + y^2$, h = 0.1, x_0=0, y_0=1.

$k_1 = h.f(x_0, y_0)$,

= 0.1 f(0,1)

= 0.1000

$k_2 = h.f(x_0 + \frac{h}{2}, y_0 + \frac{k_1}{2})$,

= 0.1f(0.05,1.05)

= 0.1152

$k_3 = h.f(x_0 + \frac{h}{2}, y_0 + \frac{k_2}{2})$,

= 0.1 f(0.05,1.0576)

= 0.1168

$k_4 = h.f(x_0 + h, y_0 + k_3).$

= 0.1 f(0.1,1.1168)

= 0.1347

and $k = \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 0.1165$

Hence $y(0) = y_0 + k$

= 1.1165.

Now $x_1 = x_0 + h = 0 + 0.1 = 0.1$

$y_1 = 1.1165,$

h = 0.1.

Again, $k_1 = h.f(x_1, y_1),$

= 0.1 f(0.1, 1.1165)

= 0.1347

$k_2 = h.f(x_1 + \frac{h}{2}, y_1 + \frac{k_1}{2}),$

= 0.1f(0.15, 1.1838)

= 0.1551

$k_3 = h.f(x_1 + \frac{h}{2}, y_1 + \frac{k_2}{2}),$

= 0.1 f(0.05, 1.194)

= 0.1576

$k_4 = h.f(x_1 + h, y_1 + k_3).$

= 0.1 f(0.2, 1.2741)

= 1.823

and $k = \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 0.1571$

Hence $y(0.2) = y_1 + k$

= 1.1165 + 0.1571

= 1.2736.

The required solution, $y = 1.2736$ at $x = 0.2$.

KEY WORDS

Keywords: Quadrature, Cubature, Definite Integral, Derivative, Polynomials, Slope, Tangent, Mid-Point, Taylor- Series.

LEARNING ACTIVITIES

a) Fill in the blanks:

1) The trapezoidal rule is a method for finding an approximate value for a________.

2) The _______ can also be called Runge-Kutta method of first order.

b) State whether true or false:

1) *quadrature rule* is an approximation of the definite integral of a function,

2) Simpson's rules generalize the trapezoidal rule to use more than two points per interval,

ANSWER TO LEARNING ACTIVITIES

a) Fill in the blanks:

1) Definite integral

2) Euler's method

b) State whether true or false:

1) true

2) false

MODEL QUESTIONS

1. Use Trapezoidal Rule to evaluate:

$$\int_1^5 x^2 + 2x \; dx.$$

Given that

X	1	2	3	4	5
F(x)	3	8	15	24	35

2. Use Simpson's One-third Rule to evaluate:

$$\int_0^1 \frac{dx}{1+x}$$

Correct to three decimal, taking h = 0.25.

3. Apply Simpson's $\frac{3}{8}$ rule to evaluate the following:

$\int_0^6 u_x dx,$ given that

x	0	1	2	3	4	5	6
u_x	0.146	0.161	0.176	0.190	0.204	0.217	0.230

5. What do you know about the Gaussian Quadrature?

6. Use Euler's Method to approximate y when $x = 0.5$, given that $y' = 2x^2 + y,$ with y = -1 fox x =0.

7. Use Euler's Improved Method to solve $\frac{dy}{dx} = -2x^2 y$ for $x = 0.6$, and h=0.2 with the boundary condition y = 1 when x =0.

8. Use the Modified Euler's Method, Solve numerically the $\frac{dy}{dx} = x^2 + y$ with initial condition y=1, x =0 for range $0 \le x \le 0.6$ in steps of 0.2.

9. Use Runge-Kutta Method of fourth order to solve $dy/dx = (y-x)/(y+x)$ with $y(0) = 1$ at $x = 0.2, 0.4$.

10. Discuss various types of Runge-Kutta Method.

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